An Introduction to S and The Hmisc and Design Libraries

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Chapter 1

Introduction

1.1 S, S-PLUS, R, and Source References

S-PLUS and R are supersets of the S language¹, an interactive programming environment for data analysis and graphics. Insightful Corporation in Seattle took the AT&T Bell Labs S code and enhanced it producing many new statistical functions and graphical interfaces. In this text we use S to refer to both S-PLUS and R languages.

S is a unique combination of a powerful language and flexible, high-quality graphics functions. What is most important about S is that it was designed to be extendable. Insightful, AT&T (now Lucent Technologies), and a large community of S-PLUS users and R developers and users are constantly adding new capabilities to the system, all using the same high-level language. S allows users to take advantage of an explosion of powerful new data analysis and statistical modeling techniques. The richness of the S language and its planned extendability allow users to perform comprehensive analyses and data explorations with a minimum of programming. As an example, S functions in the Design library (see Chapter 9) can perform analyses and make graphical representations that would take pages of programming in other systems if they could be done at all:

 $^{^{1}}$ S, which may stand for *statistics*, was developed by the same lab that developed the C language.

```
# Fit binary logistic model without assuming linearity for age or
# equal shapes of the age relationship for the two sexes
# Represent age using a restricted cubic spline function with 4 knots
# This requires 3 age parameters per sex. Model has intercept + 6
# coefficients. x=T, y=T causes design matrix and response vector to
# be stored in the fit object f. This allows certain residuals to be
# computed later, and it allows the original data to be re-analyzed
# later (e.g., bootstrapping and cross-validation)
f \leftarrow lrm(death \sim rcs(age,4)*sex, x=T, y=T)
# Test for age*sex interaction (3 d.f.), linearity in age (4 d.f.),
# overall age effect (6 d.f.), overall sex effect (4 d.f.),
# linearity of age interaction with sex (2 d.f.)
anova(f)
# Compute the 60:40 year odds ratio for females
summary(f, age=c(40,60), sex='female')
# Plot the age effects separately by sex, with confidence bands
plot(f, age=NA, sex=NA)
# Validate the model using the bootstrap - check for overfitting
validate(f)
# Draw a nomogram depicting the model, adding an axis for the
# predicted probability of death
nomogram(f, fun=plogis, funlabel='Prob(death)')
# Get predicted log odds of death for 40 year old male
predict(f, data.frame(age=40,sex='male'))
# Make a new S-Plus function which analytically computes predicted
# values from the fitted model
g \leftarrow Function(f)
# Use this function to duplicate the above prediction for 40 year old male
```

By making a high-level language the cornerstone of S, you could say that S is designed to be inefficient for some applications from a pure CPU time point of view. However, computer time is inexpensive in comparison with personnel time, and analysts who have learned S can be very much more productive in doing data analyses. They can usually do more complex and exploratory analyses in the same time that standard analyses take using other systems.

In its most simple use, S is an interactive calculator. Commands are executed (or debugged) as they are entered. The S language is based on the use of functions to perform calculations, open graphics windows, set system options, and even for exiting the system. Variables can refer to single-valued scalars, vectors, matrices, or other forms. Ordinarily a variable is stored as a vector, e.g., **age** will refer to all the ages of subjects in a dataset. Perhaps the biggest challenge to learning S for

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g(age=40, sex='male')

long-time users of single observation oriented packages such as SAS is to think in terms of vectors instead of a variable value for a single subject. In SAS you might say

```
PROC MEANS; VAR age; *Get mean and other statistics for age;
DATA new; SET old;
IF age < 16 THEN ageg='Young'; ELSE ageg='Old';</pre>
```

The IF statement would be executed separately for each input observation. In contrast, to reference a single value of age in S, say for the 13^{th} subject, you would type age[13]. To create the ageg variable for all subjects you would use the S ifelse function, which operates on vectors²:

The assignment operator \leftarrow is typed as <-.

To show how function calls can be intermixed with other operations, look how easy it is to compute the number of subjects having age < the mean age:

In S you can create and operate on very complex objects. For example, a flexible type of object called a *list* can contain any arbitrary collection of other objects. This makes examination of regression model fits quite easy, as a "fit object" can contain a variety of objects of differing shapes, such as the vector of regression coefficients, covariance matrix, scalar R^2 value, number of observations, functions specifying how the predictors were transformed, etc.

S is object oriented. Many of its objects have one or more classes, and there are generic functions that know what to do with objects of certain classes. For example, if you use S's linear model function lm to create a "fit object" called f, this object will have class 'lm'. Typing the commands print(f), summary(f), or plot(f) will cause the print.lm, summary.lm, or plot.lm functions to be executed. Typing methods(lm) or methods(class='lm') will give useful information about methods for creating or operating on lm objects.

Basic sources for learning S are the manuals that come with the software. Another basic source for learning S (and hence, S-PLUS) is a book called the *New S language* (a.k.a. "the blue book"), by Becker, Chambers and Wilks (1988). One step above the previous one is Chambers and Hastie (1992). Good introductions are Spector (1994) and Krause and Olson (2000). Other excellent books are Venables and Ripley (1999, 2000). Ripley has many useful S functions and other valuable material available from his Web page (http://www.stats.ox.ac.uk/~ripley/)³. A variety of manuals come with S-PLUSand R, from beginner's guides to more advanced programmer's manuals. Also see F.E. Harrell's book REGRESSION MODELING STRATEGIES (which has long case studies using S with commands and printed and graphical output), and other references listed in the bibliography. Another source of help are the S-news and R-help mailing lists (see biostat.mc.vanderbilt.edu/ rms).

Although not exclusively related to S and much of the material related to S packages is out of date, the statlib Web server lib.stat.cmu.edu can provide specific software for some problems.

²Note that a missing value for age in SAS would result in the person being categorized as 'Young'. In S the result would be a missing value (NA) for such subjects.

 $^{^{3}}$ Venables and Ripley's MASS S library has a wide variety of useful functions as well as many datasets useful for learning both biostatistical methods and S.

Also consult Insightful's Web page http://www.insightful.com. The AT&T / Lucent Technologies Web page (http://www.research.att.com/areas/stat/) points to many valuable technical reports related to the S language. The "Visual Demo", available from the Help button in Windows S-PLUS is a helpful introduction to the system.

We will concentrate on using S from a Linux or UNIX workstation or Windows S for Microsoft Windows or NT. When we do not distinguish between the two platforms, most of the commands described will work exactly the same in both contexts.

1.1.1 R

R is an open-source version of the S language (strictly speaking R uses a language that is very compatible with but not identical to S). R runs on all major platforms including running in native mode on some Macintosh operating systems. All of R's source code is available for inspection and modification. The system and its documentation is available from http://www.r-project.org. The Hmisc and Design libraries are fully available for R. Almost all of the command syntax used in this book can be used identically for R. There are many subtle differences in how graphical parameters are handled. R uses essentially Version 3 of the S language but with different rules for how objects are found from inside functions when they are not passed as arguments.

R has no graphical user interface on Linux and UNIX and only a rudimentary one on Windows. It lacks many of the Microsoft Office linkages and data import/export capabilities that S-PLUS has. It has most of the functions S-PLUS has, however. R runs slightly faster than S-PLUS for certain applications (especially highly iterative ones) and provides easy-to-use functions for downloading and updating add-on libraries (which R calls "packages"). As R is free, it can readily be used in conjunction with web servers. For a software developer, R's online help files are somewhat better organized than those in S-PLUS.

1.2 Starting S

1.2.1 UNIX/Linux

For now, we will discuss the use of S interactively. Before you start S, you should have created a directory where you will keep the data and code related to the particular project. For instance, in UNIX from an upper level directory, type

```
mkdir sproject
cd sproject
```

Next type

mkdir .Data

At this point you may want to set up so that S-PLUS does not write to an ever-growing audit file. The .Audit file accumulates a file of all S-PLUS activity across sessions. As this file can become quite large, you can turn it off by forming a new empty .Audit using touch .Data/.Audit, and setting the file to be non-writable using chmod -w .Data/.Audit.

Now you're ready to invoke S-PLUS.

1.2. STARTING S

```
Splus
Splus
S-PLUS : Copyright (c) 1988, 1995 MathSoft, Inc.
S : Copyright AT&T.
Version 3.3 Release 1 for Sun SPARC, SunOS 4.1.x : 1995
Working data will be in .Data
>
```

If you had not created a .Data (in what follows assume the name is _Data for Windows) directory under your project area, S-PLUS would have done it for you, but it would have placed it under your home directory instead of the project-specific directory. Creating .Data yourself results in more efficient management of your data, since (for now) everything will be stored *permanently* under .Data.

In Linux/UNIX, R is invoked by issuing the command R at the shell prompt. R data management is discussed in Section 4.2.

While in S, you have access to all the operating system commands. The command to escape to the shell is !. So, if you want a list of the files in your .Data directory, including hidden files, creation date and group ownership, you could type:

```
> !ls -lag .Data
total 90
drwxr-xr-x 2 cfa
                       staff
                                    1024 Jun 18 10:28 .
drwxr-xr-x 7 cfa
                       staff
                                    1536 Aug 11 1992 ..
-rw-r--r--
           1 cfa
                       staff
                                   85135 Jun 18 10:28 .Audit
-rw-r--r--
          1 cfa
                       staff
                                     132 Feb 14 1992 .First
                                      16 Jun 18 10:10 .Last.value
-rw-r--r-- 1 cfa
                       staff
-rw-r--r-- 1 cfa
                       staff
                                      64 May
                                             5
                                                 1992 .Random.seed
                       staff
                                              5
                                                 1992 freqs
           1 cfa
                                     229 May
-rw-r--r--
-rw-r-r--
           1 cfa
                       staff
                                      24 May
                                              5
                                                 1992 i
-rw-r--r--
           1 cfa
                       staff
                                  520431 Nov 12 1992 impute.dframe
```

In R, use the system function to issue operating system commands. In either R or S-PLUS you can use the Hmiscsys command.

Notice the file called .First. Its purpose is similar to that of an autoexec.sas, that is, it executes commands that you want done every time you start S. More on it later. (You could also have a .Last as well, for things you want S to do when you leave the system). Another way to execute operating system commands is to type unix("command"). The unix command is used more frequently in a programming environment.

1.2.2 Windows

Windows users first need to decide whether they want to put all objects created by S-PLUS in one central .Data⁴ directory or in a project-specific area. The former is OK when you are first learning the system. Later it's usually best to put the data into a project-specific directory. That way the directory stays relatively small, is easier to decide which objects can be deleted when you do spring cleaning, and you can more quickly back up directories for active projects. Users can manage

⁴In S-PLUS 2000 or earlier on Windows, .Data is _Data.

multiple project .Data directories using the *Object Explorer* in S-PLUS(see Section 4.2.3), but this method alone does not do away with the need for the Start in or current working directory to be set so that the File menu will start searching for files with your project area. Defining the Start in directory also allows S-PLUS commands that read and write external files (e.g., source, cat, scan, read.table) to easily access your project directory and not some hidden area. Note that S-PLUS 6 has a menu option for easily changing between project areas.

The existence of the current working directory is what distinguishes S from Microsoft Word or Excel, applications that can be easily started from isolated files. These applications do not need to link binary data files with raw data files, program files, GUI preference files, graphics and other types of objects. Therefore you do not need to create customized Windows shortcuts to invoke Word, Excel, etc., although Microsoft Office Binder can be used to link related files when the need arises.

The best way to set up for using Windows S-PLUS is to use My Computer or Explorer to create a shortcut to S-PLUS from within your project directory (if you don't have a project directory you can create one using My Computer or Explorer). Right click and select New ... Shortcut. Then Browse to select the file where Splus is stored. This will be under the cmd directory (under something like splus or splusxx) and will have the regular S-PLUS icon next to it. After creating the basic default short cut, right click on its icon and select Properties. In the Command line: box click to the right of Splus.exe and add something like S.DATA=.\.Data S_CWD=. . In the Start in box type the full path name of your project directory, e.g. c:\projects\myproject. By specifying S_CWD and S_DATA, S-PLUS will use a central area such as \splusxx\users\yourname for storing the _Prefs directory. _Prefs holds details about the graphical user interface and any changes you may have made to it such as system options. As _Prefs is about 100K in size, this will save disk space when you have many project, and let settings carry over from one project to another. If you want a separate _Prefs directory in each project area, substitute S_PROJ=. for S_CWD and S_DATA in the shortcut's command line.

Creation of the S-PLUS shortcut only needs to be done once per project (for S-PLUS 6 you may not need to do it at all). Then to enter S-PLUS with everything pointed to my project, click or double-click on the new S-PLUS icon. Depending on how your default Object Explorer is set up (see Section 4.2.3), once you are inside S-PLUS you will sometimes need to tell the Object Explorer where your .Data area is located so that its objects will actually appear in the explorer. Right mouse click while in the Object Explorer left pane, and select Filtering. Then click on your .Data area in the Databases window and click OK.

To quit S, simply type q() from the command line (i.e., after the > prompt), or click on File \rightarrow Exit under Windows. Do not exit by clicking on the X in the upper right corner as this may not close all of the files properly.

To execute DOS commands while under S-PLUS use the dos function or !. Under R use system(), and under the Hmisc library use sys() on any platform. For example, you can list the contents of the current working directory by typing !dir. To execute Windows programs, use the win3 function. The Hmisc library comes with a generic function sys that will issue the command to UNIX or DOS depending on which system is actually running at the time.

See Chapter 13 for methods of running S in batch mode.

1.3 Commands vs. GUIs

Windows S-PLUS is built around a menu-based point-and-click graphical user interface. This kind of interface is especially useful for analysts who use S less than once per week as there are no commands to remember. However, relying solely on the GUI has disadvantages:

- 1. You can't do simple computations such as $\sqrt{5}$.
- 2. You may want to do further calculations on quantities computed by using a menu or dialog box, but the dialogs are designed to produce only a single result. If for example you want to compute 2-sided *P*-values for a series of *z*-statistics, the distributions dialog box may only provide 1-tailed probabilities.
- 3. There are many commands and options that have not been implemented in the GUI.
- 4. If you produce a complete analysis and then new data are obtained, you will have to re-select all the menu choices to re-run the analysis⁵.

It is difficult to decide how to learn S-PLUS because of the availability of both the graphical and the command interface. Because of the richness of the commands, the fact that GUIs are not available for add-on libraries, and the ability to save and re-use commands when data corrections or additions are made, we will emphasize the command orientation. To introduce yourself to the GUI approach, invoke the Visual Demo from the Help menu tab while S-PLUS is running, or from the S-PLUS program directory. At first, go through the Data Import, Object Explorer, Creating a Graph, and Correlations demonstrations. Also read Chapter 2 of the online *S-PLUS User's Guide* and go through the Tutorial in Chapter 3. To access built-in example datasets for the tutorial, press File ... Open and look for the Examples object explorer file (.sbf file) in for example the \splusxx\cmd directory.

1.4 Basic S Commands

In its simplest form, the S command window serves as a fancy hand calculator. In the examples below S expressions are entered after the command prompt (>). For Windows S-PLUS you must first open the Commands window by clicking on its icon, which looks like:

> >x|

Results are displayed following the command line. Results are prefaced with a number in brackets that indicates the element number of the first numeric result in each line. As the following commands produce single numbers, these element numbers are not useful. Later we will see that when a long series of results spanning several lines is produced, these counters are useful placeholders. Also note that comments (prefaced with #) appear below.

> 1+1

[1] 2

 $^{{}^{5}}$ It is possible to save the commands produced by the dialogs and re-run these, but not all commands will run properly in non-interactive mode, and the automatically generated commands are verbose.

```
> 1+2*3+10 # note multiplication done before addition
[1] 17
> sqrt(16)
[1] 4
> 1+2^3
           # note exponentiation (2 to the 3rd power) done first
[1] 9
> 1+2^3*7 # exponentiation done first, addition last
[1] 57
> 2*(3+4)
[1] 14
> 2*(3+4)^2
[1] 98
> x \leftarrow 4 # store 4 in variable x
> sqrt(x)-3/2
[1] 0.5
```

Even though S is useful for temporary calculations such as those above, it is more useful for operating on variables, datasets, and other objects using higher-level functions for plotting, regression analysis, etc.

The following series of S commands demonstrate a complete session in which data are defined, a new variable is derived, two variables are displayed in a scatterplot, two variables are summarized using the three quartiles, and a correlation coefficient is used to quantify the strength of relationship between two variables.

```
> # Define a small dataset using commands rather than the usual
> # method of reading an external file
       <- c(6, 5, 4, 8, 10, 5)
> Age
> height <- c(42, 39, 36, 47, 51, 37)
> Height <- height*2.54  # convert from in. to cm.
> options(digits=4)
                          # don't show so many decimal places
> Height
                          # prints Height values
[1] 106.68 99.06 91.44 119.38 129.54 93.98
> plot(Age, Height)
> quantile(Age, c(.25,.5,.75))
 25% 50% 75%
   5 5.5 7.5
> quantile(Height, c(.25, .5, .75))  # also try summary(Height)
   25% 50%
              75%
 95.25 102.9 116.2
> cor(Age, Height)
[1] 0.9884
> cor.test(Age,Height)
   Pearson's product-moment correlation
data: Age and Height
t = 13.03, df = 4, p-value = 0.0002
alternative hypothesis: true coef is not equal to 0
sample estimates:
   cor
```

8

0.9884

1.5 Methods for Entering and Saving S Commands

Once can choose from many approaches for developing S code, entering code interactively, and saving code that runs successfully. A few of these are as follows.

- 1. You can enter commands to S one at a time, directly at the command prompt. Command recall and editing (using ↑ and ↓ keys and within-line editing through the use of the Home and End keys on Windows, for example) can be of great help in correcting statements. Typing Enter while the cursor is anywhere inside the command will cause that line to be executed.
- 2. Commands can be written in an editor window (Notepad, Emacs, Xemacs, Word, Xedit, PFE, WinEdt, UltraEdit, NoteTab, etc.) and then you can highlight/copy/paste desired commands into the S command window. You can also save the file every time you edit it, and bring it into S using the source command. You can save typing by doing something like:

See Section 1.5.1 for details on file name specification.

- 3. You can run the Emacs or Xemacs ESS package with its own interactive S window (especially in Linux/UNIX) to edit the code in an Emacs window and easily execute parts of the code.
- 4. After entering commands interactively, selected commands (and possibly their output) can be highlighted in the S command window and pasted into an editor window.
- 5. After entering commands interactively, the S History log can be copied to a file.
- 6. If your code is contained in an S function, you can have S edit the function.

```
myfunction \leftarrow edit(myfunction)
```

You may want to override the default editor, using options (editor = 'editorname'). ⁶Under Windows you can also specify the editor using Options ... General Settings ... Computations. You can also use the edit function to edit objects. This is especially handy for character

⁶For Windows Emacs you would use for example options(editor='gnuclientw'). This will cause the Emacs server (assuming Emacs had already been invoked before running the edit command) to open a new buffer containing the character representation of the object being edited, but to not return control to S until the buffer has been closed using for example Ctrl x #.

strings. In the following example, the **levels** of a categorical variable are changed interactively:

A major problem with the use of edit is that if a function contains syntax errors you will lose any changes made.

7. The fix function is an easier to use version of edit for editing functions and other objects:

| fix(myfunction) | # | assigns result to myfunction |
|--|---|---|
| <pre>fix() # edit myfunction again -</pre> | | edit myfunction again - also allows |
| | # | editing of file used in previous invocation |
| | # | of fix when file contained syntax errors |

When first learning S, method 1 is very expeditious. After learning S, method 2 has some advantages. One of these is that multiple-line commands that are not part of functions can easily be re-executed as needed. Windows S-PLUS has a builtin script editor which includes a facility for syntax checking code before it is submitted for execution. It also provides for easy submission of selected statements for execution after they are highlighted in the script editor.

One of the advantages of saving all the S code in a file is that the program can be run again in batch mode if the data or some of the initial commands change.

For managing analysis projects we have found it advantageous to have a "History" file in each project directory, where key results and decisions are noted chronologically. The History file can be constructed by copying and pasting from a batch output listing file or from the command window if using S-PLUS interactively. Other options for saving pieces of output include the sink function described in Section 3.5.4, and running the program in batch mode as described in Section 13.1.

As alluded to above, Windows S-PLUS has a new option for entering and editing code and saving results. You can open an existing "script" file (suffix .scr) by clicking on File : Open... or start a new one by clicking on File : New. You can submit code for execution using the F10 key. If you highlight code, F10 will cause only the highlighted code to be executed. Otherwise, the entire program will be executed. You can also highlight a function name (if it is a built-in function), right click, and select Help to see that function's documentation. By default, results will be displayed in a lower part of the window showing your code. You may want to drag the horizontal bar separating the program from its output to allow more space for the output window. You can control where results are outputted by clicking on Options then Text output routing. One place to store output is a Report window, which can be saved to a file in rich text format (rtf). Unlike the lower half of the script program window, the report window has a scroll bar that makes it easy to show analyses done much earlier. After clicking on Options : Text output routing : Report click on Window Tile Vertical to see the report window alongside the program window. Another advantage of the report window is that you can copy from the graph sheet into the report.

If you want to store a program you've edited in the script program window click on File : Save or File : Save As. If you do use a suffix in the file name box, the suffix will be .scr. If you name a suffix such as .s, that suffix will be used instead. If you like .s to denote S programs as many users do, you will have to click on File : Open then select All Files to view non-.scr files. In S-PLUS for Windows, the Script editor does bracket, brace, and parenthesis matching and context-sensitive indenting. By default, it will also type the matching right brace when you type a left brace.

Those who want commands executed immediately (without hitting F10) should open a command window. The output from commands can be interspersed with the commands or they can be directed to a report window.

1.5.1 Specifying System File Names in S

In UNIX, directory levels are separated using / both at the system prompt as well as inside S. In Windows, file names use $\$ outside of S (e.g., when defining shortcuts or in pop-up windows from the S-PLUS File ... menu). Inside Windows S you must use $\$ inside quoted file names. You can also use / (single slash), as S is kind enough to translate / to $\$. $\$ is used instead of $\$ because inside a quoted character string $\$ is considered an "escape" character that modifies the meaning of another character. For example, the character string \n is a newline character.

1.6 Differences Between S and SAS

Four of the most important distinctions between S and SAS are (1) the S language was designed to be extendable; (2) it is very easy for users to write their own S functions; (3) SAS graphics require a large amount of programming, are non-interactive, are inflexible, and have poor appearance; and (4) SAS is much more efficient than S for analyzing very large databases. On (1), S makes it very easy for users to add to the basic S language. For example, they can add new operators and new data attributes such as comment attributes for variables or data frames and flags to mark that some values are imputed.

Regarding (2), when SAS first began to be widely used around 1969, it was very easy for users to write their own procedures in Fortran. They could easily define the notation to be used for their new PROC statement, and read SAS datasets using Fortran. Many users wrote SAS procedures, including Harrell's PROCs PHGLM and LOGIST, which gave SAS the capability to fit logistic and Cox regression models in 1978 and 1979, respectively. In the late 1980's, SAS converted to a new mode for writing procedures, first in PL/I then in C. The interface became much more difficult to program, and in fact SAS started selling the interface as a separate product (the SAS Toolkit). So not only did all old SAS procedures written by users all over the U.S. become obsolete, but users had great difficulty in writing add-on procedures. On the other hand, the most basic S language texts tell you how to write your own functions, in the same language that S and S developers use. Within your own functions you can also call Fortran or C subroutines extremely easily. As a result, modern statistical methods are available in S long before they become available in SAS if at all.

In terms of ease of learning, anecdotal reports indicate that S is easier to learn than SAS for users who don't already know SAS. For previous SAS users, the vector and interactive programming orientation of S may take a bit of getting used to.

The following table compares SAS with S in several areas.

| Table | 1.1. <u><u> </u></u> | | UJ SAS | unu S | |
|-------|-------------------------|-------------|--------|-------|--|
| Table | 1 1. | Comparisons | ofGAG | and C | |

| Feature | \mathbf{SAS} | S | | |
|---|--|--|--|--|
| Numeric value storage | Floating point, 3-8 bytes | Integer, float single, float double (4, 4, 8 bytes) | | |
| Character value storage | 1-200 bytes, fixed length (although dataset may be compressed) | no limit, variable length | | |
| Variable names | Up to 8 letters (31 for Version 8), case-insensitive (case-sensitive for V8), special character possible: - | Any length, case-sensitive, special character possible: . | | |
| Variable labels | Up to 40 letters (256 for V8) | Any length, user-defined attribute | | |
| Value labels | Created by PROC FORMAT, stored separate from data | Intrinsic attribute stored with data in factor variables | | |
| Standard missing values | ., check using x=. | NA, check using is.na(x) | | |
| Special missing values | Values .A,,.Z, part of standard language | User-added attributes created auto- matically by sas.get function | | |
| Missing val- ues in logical expressions | Treated as the smallest number, log- ical expression will never result in missing | Uses correct rules, e.g., $T \ \ NA \ {\rm is} \ T,$ $F \ \ NA \ {\rm is} \ NA, \ NA \ < \ 50 \ {\rm is} \ NA$ | | |

=

_

| Feature | \mathbf{SAS} | \mathbf{S} |
|---|--|---|
| User-defined attributes | Not possible | Added at will. Examples: $comment(x) \leftarrow `Variable was$ corrected 4/1/97' is.imputed(x), partial dates, name of image file containing page of data form where variable was entered |
| Processing of Ob- servations | Record by record | As vectors or matrices |
| Dataset format | dataset = rectangular table | data frame = list of vectors and ma- trices; can attach attributes to data frame |
| By-processing | Run PROC SORT then use BY state- ment on PROC to group analysis | Execute functions in a loop, for dif- ferent subsets (subscripts) of obser- vations, or use tapply or related functions |
| Post-processing of analysis output | Some printed output not available in procedure output datasets (Out- put Delivery System does help). Hard for user to derive secondary estimates/simulate/bootstrap. | All calculated values are stored in objects created by functions. Easy to compute other estimates or feed output to bootstrap procedure. |
| Handling huge datasets (e.g., 100,000 obser- vations on 50 variables) | Limited only by disk space | Limited by memory. Will be very slow if data must be stored in virtual memory that is swapped to disk. |

| Feature | SAS | S |
|------------------------------|---|--|
| Speed | Linear in dataset size | Faster for small-moderate datasets; slower for large ones if use virtual RAM |
| Merging | General, efficient | General, slower |
| Inputting Raw Data | Flexible, reads non-standard data formats | Flexible for ASCII files |
| Processing steps | Separate DATA and PROC steps exe- cuted in batch mode | Line-by-line interactive, can mix data generation and analysis steps |
| User-written pro- cedures | Computational modules can be written using a separate procedure (IML). Can not mix standard PROCs using this mode. Symbolic macro language can mix PROC,DATA steps. Macro language is harder to write and is not "live". PROCs are very difficult to write, and users cannot add online help files for them. | User writes functions using stan- dard S language. No symbolic macros are needed. Commands are "live", i.e., can sense data values and attributes at time of execution. For example, the describe function has a statement like the following to give output appropriate to the type of input variable: if(is.category(x) length(unique(x)) < 20) table(x) else quantile(x). Easy to call C or Fortran routines from S functions. User-written online help looks builtin. |
| Vector and matrix operations | Available while running PROC IML | Intrinsic part of language |

| Feature | SAS | S |
|---|--|---|
| System Source Code | Not available | Visible for most functions by typ- ing function name. Can learn from, adopt, modify, correct system func- tions. |
| Graphics | non-interactive, difficult to pro- gram, restrictive, ugly | interactive and batch, best statistical graphics available |
| Handling of cate- gorical variables in regression models | Some procedures allow CLASS state- ment and generate dummy vari- ables; many do not. | Dummies always automatically gen- erated |
| Nonlinear effects in models | One or two procedures will generate quadratic terms; most require user to code nonlinear component vari- ables. | All models allow general transfor- mations of predictors directly in the model formula |
| Interaction effects | Few PROCs will generate these; users must code products (in DATA step) and test them manually | Automatic |
| Tests of nonlin- earity and pooled interaction effects | Must be done manually | Automatic when using the Design library |
| Plot how each predictor is represented in model | Must create auxilliary datasets and program | Single statement using Design |

| Feature | SAS | S |
|--|--|--|
| Robust covari- ance estimation for fitted models | Macros for "sandwich" estimator available for certain models | "Sandwich" or bootstrap, with clus- ter sampling adjustment, available using a single statement with Design |
| Model validation | Not available | Single statement using Design |
| Computing Predicted Values | Must create dataset containing pre- dictor settings, add to original dataset, and re-run model fit | If saved result of fitting function ("fit object") can obtain predictions for any desired predictor settings us- ing predict(fit,) or using the Design library's Function function |
| Graphical sum- mary of model | Not available | Effect plots and nomograms with Design |
| Missing value im- putation | PROC MI for linear imputations models with normal distributions | General method using Hmisc's aregImpute and impute functions |
| Bayesian infer- ence | Not available | BUGS package interfaces with S |
| Mixed models | PROC MIXED for linear models has nice features for Gaussian, binary, Poisson responses | A few models are available, includ- ing nonlinear mixed models; compu- tational properties not as good as PROC MIXED. |

| Feature | SAS | S |
|--|--|--|
| Penalized maxi- mum likelihood estimation | Ridge regression for linear Gaussian models | More general penalized MLE for lin- ear Gaussian model and binary and ordinal logistic models, with differ- ential penalization by type of term in model |
| Penalized estima- tion with variable selection | Not available | lasso function in Statlib |
| Tree models (CART) | Not available except in Enterprise Miner | rpart function and graphical representation |
| Generalized addi- tive models | Recently available | Builtin |
| Nonparametric smoothing | Extremely slow PROC IML macro; new features for V8 | Builtin, variety of smoothers |

The following table lists SAS procedures and corresponding S functions. In this table, ols,lrm,psm,bj,

| SAS Procedures | S Functions | |
|----------------------------|---|--|
| ANOVA | aov | |
| REG,GLM | lm,glm,ols,bj,manova | |
| LOGISTIC | glm,lrm | |
| LIFEREG | survreg,psm,bj | |
| LIFETEST | <pre>surv.diff,survfit,cph</pre> | |
| PHREG | coxph, cph | |
| FREQ | table,crosstabs,summary.formula | |
| | mantelhaen.test,fisher.test,chisq.test | |
| TABULATE | summary.formula | |
| MEANS, SUMMARY, UNIVARIATE | mean,var,quantile,summary,describe | |
| CORR | corr,rcorr | |
| VARCLUS | varclus | |
| PRINQUAL | transcan | |
| BY statement | <pre>tapply,by,aggregate,split,summary.formula, summarize,for</pre> | |

Table 1.2: SAS Procedures and Corresponding S Functions

and cph are from the Design library, and summary.formula, summarize, rcorr, describe, varclus, and transcan are from the Hmisc library. Other functions are built-in.

1.7 A Comparison of UNIX/Linux and Windows for Running S

The UNIX/Linux operating system is a better environment for software developers because of the wide variety of tools available⁷. UNIX/Linux is also a good choice if you are processing large databases, as it is cost-effective to have a "compute server" on your UNIX/Linux network that can be used by many users for large applications⁸. Having used both UNIX and Windows extensively, we feel that UNIX (and hence Linux) is a more efficient and reliable environment for every day S users, as UNIX window navigation is more efficient than Windows. Windows users tend to spend too much time navigating menus and Windows operates significantly slower than Linux because of the design and massive size of Windows operating systems. However, the greatest advantage of UNIX is probably that a nice system administrator would have already installed the tools you need, including Emacs, Ghostview, IATEX, and a variety of print utilities. Many versions of Linux come with all of these tools automatically. But Windows has a few advantages also: (1) ease of installing add-on S-PLUS and R libraries; (2) faster online help for S-PLUS; (3) outputting graphs in Windows

 $^{^{7}}$ Windows users can not-so-easily install versions (e.g., GNU) of many of the UNIX tools, such as a **bash** shell command window.

⁸You can also program a UNIX system to compress large databases that haven't been read in a week. That way your disks will not fill up nearly as quickly.

metafile and other formats for easy inclusion and editing using Microsoft PowerPoint or Word⁹; and (4) only the Windows version of S-PLUS has menus for doing standard analyses and graphics. S-PLUS 6 is available for UNIX, Linux, and Windows. This has resulted in a partial convergence of Linux/UNIX and Windows S-PLUS, with a more or less a common graphical user interface¹⁰.

See http://biostat.mc.vanderbilt.edu/s/howto/linux.setup.html for more information on setting up a Linux system and installing software of interest to data analysts.

1.8 System Requirements

For UNIX/Linux a minimum amount of RAM is 64MB. For PCs, 128MB is minimal. If you will be analyzing large databases (roughly speaking, > 40000 observations), you may need at least 256MB of RAM. For analyzing very large databases (say > 100000 observations), more than 256MB of RAM will usually be needed. Windows 2000 and XP use memory much more inefficiently than earlier versions of Windows, so add more RAM accordingly. RAM is cheap, so it's best to order your PC with 256MB. If you have only occasional need for more than 256MB of RAM, you may want to endure the slowness of virtual memory for those applications.

A minimum PC CPU for running Windows S-PLUS is a 400 MHz Pentium. R requires less memory to run than S-PLUS.

1.9 Some Useful System Tools

There are several system tools that can greatly assist the S user. UNIX users usually have an advantage in that their system administrator would have already installed most of the tools, and many linux packages come with all of the important tools pre-installed. For Windows users, Web addresses for obtaining the software are provided. **biostat.mc.vanderbilt.edu/EmacsLaTeXTools** has a large amount of information on obtaining an installing **Emacs**, IAT_FX, and related programs.

Emacs editor: Emacs is an incredibly powerful editor for editing text files of various types. Emacs is especially powerful for editing S code, as it has a special mode which highlights different kinds of S statements in different colors or fonts and it does indentation according to the level of nesting. It also makes it easy to check for matching parentheses, brackets, and braces. Emacs for Windows (all 32MB of it when uncompressed!) is available from ftp://ftp.gnu.org/-gnu/windows/emacs/latest. Harrell's version of the Emacs startup file (.emacs) is available from the Utilities area of the UVa Web page This .emacs file has several useful default settings for how Emacs operates. S-mode for Emacs using the ESS Emacs package may be obtained from http://software.biostat.washington.edu/statsoft/ess. S-mode can also run S-PLUS or R itself, allowing for such capabilities as object name completion in the editing window if you enter the first few letters of an object's name. This mode is known to work well under UNIX/Linux.

⁹Windows S-PLUS can output graphics directly into Powerpoint Presentation format as well as Adobe Acrobat .pdf files (see below), and R can make .pdf files. Note however that using Windows metafiles to include graphics into Microsoft Office applications frequently does not preserve all aspects of the graphics. Postscript is still the most reliable graphics format.

¹⁰This version is based on the version 4 engine of the S language, which will require some functions to be modified unfortunately. All modifications have been made in Harrell's libraries.

Windows users may find that **Xemacs** is a bit more user-friendly, and Xemacs has a menu for automatically downloading and installing packages such as ESS. Like Emacs, Xemacs can be automatically installed when you install Linux. Windows users may obtain Xemacs from www.xemacs.org.

- **Ghostview**: This is a previewer for postscript graphics and documents. It is available for Windows from http://www.cs.wisc.edu/~ghost/. Ghostview comes with Ghostscript, which can convert postscript files to .pdf files (but not as efficiently as Adobe Acrobat) among other things.
- IATEX: This system is excellent for composing technical documents and advanced tables. It is the typesetting system used to make this document, and it is used by many book publishers. An excellent commercial version of IATEX for Windows can be obtained by contacting Personal TEX Inc. at texsales@pctex.com or http://www.pctex.com. If you want to be able to produce electronic documents (e.g., .pdf files) with hyperlinks, the full TEX package from Y&Y Inc. is recommended. See www.YandY.com. Perhaps the best versions of IATEX for Windows are free versions, FPTEX by Fabrice Popineau and MikTEX, both available at http://www.ctan.org. FPTEX's DVI previewer allows postscript graphics to be displayed, assuming you have installed Ghostscript. Several tools for creating .pdf files are also included in FPTEX. See http://ctan.tug.org/tex-archive/info/lshort/english/lshort.pdf for a nice free book for learning IATEX.
- Adobe Acrobat Reader: Available from www.adobe.com, this free program nicely displays .pdf files. You can create these graphics files directly in Windows S-PLUS using the pdf.graph device function. Occasionally this will get around printer memory problems when printing complex graphs, and a few graphs can only be faithfully printed in Windows this way.
- Metafile Companion: This program, for which a free trial version is available from www.companionsoftware.com, allows you to edit Windows metafiles, a graphics format you can produce either with the dev.print function in S 3.2+ or using the File ... Export Graph dialog. Metafile Companion is one of the nicest graphics editors available anywhere. It allows you to edit any detail of the graph.
- Mayura Draw: This shareware program is a nice scientific drawing program. It can take as input an Adobe Illustrator file, which can be converted by Ghostscript from a postscript file. Using that combination of programs gives you the ability to nicely edit postscript graphs. See www.mayura.com for information about Mayura Draw.
- graphviz: This is an amazing command language from AT&T for drawing complex tree diagrams. Linux, UNIX, and Windows versions are available from http://www.graphviz.org
- Xmouse: You can make a Windows 95 mouse work like a mouse in UNIX X-windows by installing Microsoft's PCToys package and running its Xmouse program. That way when you move the mouse from an editor window to the S command window you do not need to click the left mouse button to make the S window have the mouse's focus. This really helps in copying text from the editor to S. Also, if you had to click the left mouse button, the editor window would usually disappear. For Windows 95, obtain Xmouse from the Powertoys package at www.microsoft.com/windows95/downloads/contents/wutoys/w95pwrtoysset. For

Windows 98, this functionality is in the tweakUI package that is an optionally installed component of the Win 98 installation disk. With Windows 98 tweakUI you can also specify an option to have the "currently focused on window" automatically move to the top.

- **UltraEdit**: Users who want a powerful programmer's editor that is not as comprehensive (or as large) as Emacs may want to consider buying UltraEdit (www.idmcomp.com).
- WinEdt: Next to Emacs this is probably the best editor for Windows/NT users, especially when used in conjunction with LATEX. Trial and licensed copies may be ordered from www.winedt.-com.
- NoteTab: This is a nice editor for Windows that has a flexible macro language for making the editor language-sensitive and allowing submission of code to an open window (using ctrl-space (repeat last macro)). A free version is available from www.notetab.com. Dieter Menne (<dieter.menne@menne-biomed.de>) wrote the following macros for using NoteTab with R.

```
^!FocusDoc
;Save the file if it has been modified
; ^!Save
;Select the highlighted block.
^!If ^$GetSelSize$ = 0 END ELSE SelectLines
:SelectLines
:GetSelection
^!Set %AnyText%=^$GetSelection$
;Write the selected text to a temporary file in the Windows temp. dir.
^!Set %fileName%=^$GetTmpPath$std0001.r
^!Set %fileName%=^$StrReplace(\;/;^%fileName%;True;False)$
^!TextToFile ^%fileName% ^%AnyText%
; Copy "source" to the clipboard
^!SetClipboard source("^%fileName%")
; Switch to R
^!FocusApp RGui*
;ESC to clear the Command window, paste the command, hit enter
^!Keyboard ESC
^!Keyboard CTRL+V
^!Keyboard ENTER
```

Dieter also wrote the following reg-file to start R from Windows Explorer .

REGEDIT4

[HKEY_CLASSES_ROOT\Directory\shell\Run R]

[HKEY_CLASSES_ROOT\Directory\shell\Run R\command] @="\"C:\\Program Files\\R\\rw1050\\bin\\Rgui.exe\" --internet2"

- **TeXmacs**: This is a WYSIWYG front-end to LATEX for Linux and UNIX users that gives you a full equation editor. It is available from www.math.u-psud.fr/~anh/TeXmacs/TeXmacs.html.
- PFE: A nice small and free programmers editor is PFE which may be downloaded from http://www.-lancs.ac.uk/people/cpaap/pfe/. PFE is an excellent replacement for NOTEPAD even if you just use it for viewing files. If PFE is already open and you invoke it on another file, it will add the new file to the list of files it is currently managing. Emacs can do this using its GNUCLIENT feature. To use PFE as your default editor, you can issue the S command options(editor='c:/pfe/pfe32') if pfe32.exe is stored on the c:\pfe directory, or enter the Options ... General Settings ... Computations dialog.
- Microsoft Word Damien Jolley (djolley@ariel.ucs.unimelb.EDU.AU) wrote a Microsoft Word macro that allows one to execute send highlighted code to S for execution. His macro definition follows.

```
Sub MAIN
If SelType() <> 2 Then EditSelectAll
'Select all if none current
EditCopy
SendKeys "%w1+{insert}{enter}^{F6}"
AppActivate "S-PLUS for Windows"
End Sub
```

A Word 97 version of the macro follows.

```
Public Sub MAIN()
If WordBasic.SelType() <> 2 Then WordBasic.EditSelectAll
'Select all if none current
WordBasic.EditCopy
WordBasic.SendKeys "%w1+{insert}{enter}^{F6}"
WordBasic.AppActivate "S-PLUS for Windows"
End Sub
```

To quote from Damien: "I have this stored as a macro which I can execute from a user-defined button on the Toolbar. So, when I'm ready to test my bit of code, I just click the button, and Windows switches over to S-PLUS, copies the code into the S-PLUS command buffer and execution takes place immediately. I use ALT-TAB to return to Word either to fiddle with the code or to save it to a text file". To enter the macro, record and then edit a macro. You start the recorder and enter a random command, then stop the recorder and give the macro a name. Then edit it to make the real macro.

John Miyamoto jmiyamot@u.washington.edu has a series of Word 6 macros for interfacing with S-PLUS. These macros are available from the Utilities area under Statistical Computing Tools on the UVa Web page.

1.9. SOME USEFUL SYSTEM TOOLS

JED This is a nice small version of Emacs available from John Davis at http://space.mit.edu/~davis/jed.html.

Chapter 2

Objects, Getting Help, Functions, Attributes, and Libraries

2.1 Objects

In SAS, one has several concepts which refer to different types and characteristics of data, like data files, data views, data catalogs, format catalogs, libraries, etc. You get results from these data by using a PROC step. S has different entities representing data such as vectors, factors, matrices, data frames, lists, etc. These entities have different characteristics called *attributes* such as names, class, dim, dimnames etc., and we get results by applying *functions* to them. In general, any entity in S is designated by the general name of an *object*.

The names of objects in S can be of any length, and can contain digits, mixtures of lower and upper case letters, and periods. Names may not contain underscores and may not start with a digit. In some cases you will want the names to be very descriptive (e.g., **age.years**) but in other cases it's best to use a short name (e.g., **age**) and then to assign a longer label as an attribute ¹.

Names in S are case-sensitive, so that vectors **age** and **Age** would refer to two different objects. This can be handy for distinguishing between various versions of the same basic information. For example, **age** might refer to the original age variable whereas **Age** might refer to age values after certain data corrections or missing value imputations.

2.2 Getting Help

Suppose we want to get help on a function, and see if it has any options that we may want to use. There are several ways to do this. A very simple one is to type **?mean** (or whatever the name of the

¹This can be done using the label function which is in the Hmisc library described below, e.g., label(age) \leftarrow 'Age in years'. When using the sas.get function to convert SAS datasets to S data frames, SAS labels are automatically carried to S in this fashion.

function is). Equivalently, we could type help(mean). In the case that the function contains special characters, its name should be enclosed in quotation marks, thus help("%*%") means help for the matrix-product function.

```
>?mean
Mean Value (Arithmetic Average)
DESCRIPTION:
      Returns a number which is the mean of the data.
                                                        A frac-
      tion to be trimmed from each end of the ordered data can
      be specified.
USAGE:
      mean(x, trim=0, na.rm=F)
REQUIRED ARGUMENTS:
      numeric object. Missing values (NAs) are allowed.
x:
OPTIONAL ARGUMENTS:
trim:
         fraction (between 0 and .5, inclusive) of values to be
      trimmed from each end of the ordered data. If trim=.5,
      the result is the median.
na.rm:
         logical flag: should missing values be removed before
      computation?
VALUE:
       (trimmed) mean of x.
DETAILS:
      If x contains any NAs, the result will be NA unless
      na.rm=TRUE.
                   If trim is nonzero, the computation is per-
      formed to single precision accuracy.
```

When you use either of these two forms of help, the system looks for a file in some directory and then displays the help file. This means that a window will pop up with options to print the help file, search for character strings, etc.² If you are running on a UNIX workstation, you may want to initiate the interactive help system. Type help.start() and a window listing all functions and categories of functions will appear. Just click on the one you want help about, and a new window will pop-up with help specifically on that function. You can then look at it, close it to keep it around or send it to the printer. With this method you can also type something like regres* in the topic field of the help window, to get a list of all functions which start with 'regres'. The disadvantage is that this is slower. To quit the window type help.off().

A third way, if you don't want full help but to just be reminded of what the arguments to the function are, is to use the **args** function built in to S.

²Under UNIX X-Windows it is beneficial to use e.g. options(pager='xless') to use a full-screen pop-up window instead of the system default in which the less command is run inside of the S command window.

2.2. GETTING HELP

```
> args(mean)
function(x, trim = 0, na.rm = F)
```

The function has three arguments, x for the vector of which we want the mean, trim= if we want trimmed means, na.rm=, to remove missing values. The defaults are trim=0 and na.rm=F. Here T is the logical true value, so we interpret na.rm=T as saying that the na.rm argument is turned "on." If you name the arguments, they can be given in any position. For example mean(x,na.rm=F,trim=.5). See Section 2.3 for more about functions and arguments.

You can also use names(functionname) to list the arguments, or

functionname\$argumentname to list the default argument value. A quick way to get an alphabetic listing of a function's arguments is to type

sort(names(function.name)). Note that there is an extra element with a blank name that should be ignored.

```
> sort(names(mean))
[1] "" "na.rm" "trim" "x"
```

The object orientation of S can make it difficult to know the full name of the function you are really using. For example, if you need help in plotting a logistic regression fit using the Design library, you may not know that the pertinent plot function is plot.Design. You can get a list of all of the plot methods by typing methods(plot). You can get a list of all of the methods for handling the fit object by typing methods(class=class(f)) if the fit object is f.

If you are having troubles understanding what the function does or how it is doing things, you can always look at the function itself.

```
> mean
function(x, trim = 0, na.rm = F)
{
         if(na.rm)
           x \leftarrow x[!is.na(x)]
         else if(any(is.na(x)))
           return(NA)
         if(mode(x) == "complex") {
                 if(trim > 0)
                    stop("trimming not allowed for complex data")
                 return(sum(x)/length(x))
         }
        x <- as.double(x)</pre>
         if(trim > 0) {
                 if(trim \ge 0.5)
                   return(median(x))
                 n \leftarrow length(x)
                 i1 <- floor(trim * n) + 1
                 i2 <- n - i1 + 1
                 x <- sort(x, unique(c(i1, i2)))[i1:i2]</pre>
         }
         sum(x)/length(x)
```

}

Yet another possibility is to look at the help files without even starting S-PLUS. You may find yourself in this situation if you are running a job in batch mode and want to find out why it didn't work. In UNIX it's easy to define shell programs to facilitate this, as well as to list help files associated with keywords. Under Windows, you can use Explorer or My Computer to click on a .hlp file in the main S-PLUS area or in an add-on library area (see below).

Last, but not least, consult the back of the blue book or the S-PLUS User's manual. The help here is exactly the same as the on-line help but not all functions are listed. In S-PLUS Version 4.x and later the manuals are online with some search capability.

The following is a list of major help topics for S-PLUS as it is distributed from MathSoft. This list will help in understanding the components of the system as well as how you can find a function when you don't know its name. In Windows you could click on any of these topics to see all functions related to that topic. In UNIX you use the help.start() command to put up the list of topics.

Add to Existing Plot All Datasets ANOVA Models Categorical Data **Character Data Operations** Clustering **Complex Numbers** Computations Related to Plotting Customizable Dialog functions Customizable Menu functions Data Attributes Data Directories **Data Manipulation** Data Types Dates Objects Demo Library Demonstration of S-PLUS **Deprecated Functions** Documentation **Dynamic Graphics** Error Handling Graphical Devices **High-Level** Plots Input/Output-Files Interacting with Plots Interfaces to Other Languages Library of Chapter 11 Functions from The New S Language Library of Chronological Functions Library of Drawing Functions from Programmer's Manual Library of Examples from Programmer's Manual Library of Examples from The New S Language Linear Algebra Lists Loess Objects Logical Operators

2.3. FUNCTIONS

Looping and Iteration Mathematical Operations Matrices and Arrays Methods and Generic Functions Miscellaneous Multivariate Techniques Non-linear Regression Nonparametric Statistics Optimization **Ordinary Differential Equations** Printing Probability Distributions and Random Numbers Programming Quality Control Regression Regression and Classification Trees RELEASE NOTES Robust/Resistant Techniques **Smoothing Operations** S-PLUS Session Environment Statistical Inference Statistical Models Survival Analysis Time Series Trellis Displays Library Utilities

2.3 Functions

You are starting to see that unless you are using the pull-down menu system in S-PLUS, almost everything is done by calling functions³. A function is an object in S and in many ways it can be operated on as data. Most functions have *arguments* that pass values to the function for it to work on or to specify detailed options on how it should do its work. It is common for example to pass a vector of data (representing a single variable) to a function along with scalars or other shorter vectors specifying options such as confidence levels, quantiles, plotting and printing options, etc.

Arguments are given to the function either by name or by their sequential position in the series of arguments. It is very common to specify a "major" argument without its name, in position one, then to specify "minor" arguments by name. This is because there are so many "minor" arguments and it is hard (and risky) to try to remember their order. For example, we can compute the mean **age** using the command **mean(age, na.rm=T)**, which means to compute the mean of the **age** vector ignoring missing values. We could use the equivalent statement **mean(age, , T)**, i.e., we can assign the logical "true" value (T) to the third argument to **mean**, which we can see from **mean**'s help file is the **na.rm** argument. The extra comma is a placeholder to specify that we are not specifying the

³Menu choices are actually executed by secretly calling functions.

second argument which is trim. trim will receive its default value of zero. As mentioned above, this is a dangerous method so we prefer mean(age, na.rm=T).

When we examined the help file for the mean function we saw na.rm=F in the list of arguments. This means that the default value for na.rm is F, so that na.rm will be assumed to be F if you do not specify this argument. Default values can also be vectors, lists, matrices, and other objects as the need arises. Often you will see that the default for an argument is a vector of values when the argument really needs to be a scalar. In these cases, the vector of values frequently specifies the list of possible values of the argument, with the default value listed first. For example, look at the argument list for the residuals.lm function:

```
> args(residuals.lm)
function(object, type = c("working", "pearson", "deviance"))
```

Here the type argument can take on three possibilities. If you do not specify type, 'working' residuals will be computed.

2.4 Vectors

A statement to create a vector interactively could be something like this

> x ← c(3.1,2.6,3.4,5.9,7.6)

In creating \mathbf{x} we used two S operators, the assignment statement " \leftarrow " which is read " \mathbf{x} gets ..." and the concatenation function c(). A synonym for \leftarrow is the underscore sign (_). Of course the assignment could have been written in a reversed way,

> c(3.1,2.6,3.4,5.9,7.6) \rightarrow x or > c(3.1,2.6,3.4,5.9,7.6) _ x

Two or more assignments could be made on the same line if separated by a semicolon. A line could also be split among two or more lines. Just hit **return** at the end of your line and you will get a continuation prompt "+" at the beginning of the next line, then continue typing. You can concatenate two or more existing vectors and include other data as an argument to the c() function.

```
> y \leftarrow 10.6:2.3;z \leftarrow c(x,c(1,2,3),y + y^2)
Syntax error: name ("y") used illegally at this point: z \leftarrow c(x,c(1,2,3),y y
```

Here, we forgot the comma after y on the first line.

> y \leftarrow 10.6:2.3;z \leftarrow c(x,c(1,2,3),y, + y^2,y+1)

If we want to see what's stored in the vectors **y** and **z** just type their names

```
> y
[1] 10.6 9.6 8.6 7.6 6.6 5.6 4.6 3.6 2.6
> z
```

2.4. VECTORS

| [1] | 3.10 | 2.60 | 3.40 | 5.90 | 7.60 | 1.00 | 2.00 | 3.00 | 10.60 | 9.60 |
|------|-------|-------|-------|-------|-------|------|-------|--------|-------|-------|
| [11] | 8.60 | 7.60 | 6.60 | 5.60 | 4.60 | 3.60 | 2.60 | 112.36 | 92.16 | 73.96 |
| [21] | 57.76 | 43.56 | 31.36 | 21.16 | 12.96 | 6.76 | 11.60 | 10.60 | 9.60 | 8.60 |
| [31] | 7.60 | 6.60 | 5.60 | 4.60 | 3.60 | | | | | |

There are several things to notice here. First, the operator a:b produces a sequence from a to b starting with a and adding (or subtracting) 1 to each element until you get a number greater in absolute value than |b|. (You may want to experiment to see what happens when a or b are negative). Second, we have y^2 which just squares each element of y. All functions which return a single numerical result from a single numerical argument such as exp,sqrt,sin,cos,tan,atan,log, etc. act on each element of the vector. Finally, adding a number to a vector just adds the number to each component of the vector.

What happens if we add two vectors of different length? Let's see.

When adding (or subtracting) two or more vectors of different length, the shorter vectors are recycled until they reach the length of the longest vector and then the operation is performed and a warning message is issued. Also notice that we did not assign the result of the sum, but printed it directly instead.

To list vectors left over from a previous session, use objects(). To delete them, use rm(x,y,z) where x, y and z are the vectors to be deleted. This function works in exactly the same way with objects other than vectors. You can also use the more versatile remove function to delete objects, e.g., remove(c('x', 'y', 'z')).

Next, let us do some statistics on these vectors. How many observations do we have? What is the mean? And the standard deviation?

> length(z)
[1] 35
> mean(z)
[1] 17.384
> sqrt(var(z))
[1] 26.59949

2.4.1 Numeric, Character and Logical Vectors

All elements of a vector must be of the same type, that is integers, real numbers, complex numbers, logical values (T or F), or character strings. Examples of each kind are c(3,6,9), c(1+2i,.2,-3-5.6i),(T,T,F) and c("x","y","z"). To determine what kind of vector we have, we could type mode(x) and this will return a character string telling us the kind of vector. It is also possible to assign a value to the mode of a vector forcing it to be something else.

> $x \leftarrow c(3.1, 2.6, 3.4, 5.9, 7.6)$

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```
> x
[1] 3.1 2.6 3.4 5.9 7.6
> mode(x)
[1] "numeric"
> mode(x) ← "character"
> x
[1] "3.1" "2.6" "3.4" "5.9" "7.6"
>
```

There are a number of functions to test for the mode of a vector and to change it. In general, if we try to operate on a vector whose mode is not appropriate for that kind of operation, S will automatically convert it to another kind trying to lose the least possible amount of information in the process. Thus, c(T,F)+c(3,4) yields c(4,4) (Fs are converted to zeros and Ts are converted to ones). The functions to test and change modes are

is.numeric,as.numeric
is.character,as.character
is.logical,as.logical

A useful function in the Hmisc library which may save you some typing is Cs(a,b,c,d). It is equivalent to c("a","b","c","d") but it won't work if your character strings have an _ in them (since _ is equivalent to \leftarrow).

2.4.2 Missing Values and Logical Comparisons

Missing values in numeric and logical vectors are represented by the symbol NA (not available). In general, any operation (mathematical or logical) performed on a missing value will return a missing value. The logical operators are >, >=, <, <=, ==, !=, &, |,!. Notice that the operator to test equality is == rather than =, which is reserved for named arguments to a function. ! is used for negation and & and | for logical 'and' and 'or'. Consider for instance

> x \leftarrow c(3,6,9,10,2.2,NA,NA,6.7); y \leftarrow c(1,6,9,2,NA,5.1,0,-1) > x > y > [1] T F F T NA NA NA T

The operator == is not appropriate to test for missing values. Instead, use the function is.na.

> is.na(x > y) [1] F F F F T T T F

Suppose that we have two vectors of the same length, and we want to know the joint distribution of their missing values.

> x [1] 1 1 1 NA NA 2 2 2 2 2 2 NA > y [1] 2 2 2 2 2 NA 4 NA 1 1 1 1

One way would be to use the table function

```
> table(is.na(x),is.na(y))
        FALSE TRUE
FALSE 7 2
TRUE 3 0
```

You can also tabulate all patterns of NAs using the builtin function na.pattern (but note that na.pattern was omitted from S-PLUS 2000):

```
> na.pattern(list(x,y))
00 01 10
7 2 3
```

Also see the **naclus** function described under the **varclus** function in the Hmisc library discussed below.

2.4.3 Subscripts and Index Vectors

It is possible to select subsets of a vector by *subscripting* or *indexing* its elements. This is equivalent to using a WHERE statement in SAS, but it is more flexible. The expression to use is x[i] where i could be another vector, or an expression which evaluates to a numeric, logical or character vector. In all cases, we'll think of the elements of x as being subscripted by the indexes 1:length(x) when [] is not present.

- 1. If i is a numeric vector, all its elements must be >=0 or all <=0 (NAs are allowed). Before selecting the subset, S drops all zeros from the index vector. If all elements of i are positive, then x[i] selects only those elements of x whose subscripts match the elements of i. If the elements of i are negative, then x[i] selects the elements of x whose subscript *does not match any element* in i. If the *kth* element of i is NA then the *kth* element of x[i] will be NA as well. (0s are ignored). i can be any length.
- 2. If i is a logical vector, it is indexed starting at 1 and those elements of x whose subscripts have a value of T in the corresponding index of i are selected. The same rule as in 1. apply to NAs. For this case, the length of the index vector should equal length(x).
- 3. If i is a character string (of any length), the rules are a little bit different. In this case x is required to have what's called a *names* attribute. A **names** attribute is a vector of character strings of the same length as x which effectively names each element of x. Assuming that x already has a **names** attribute, the expression x[c("a", "b")] selects the first element of x named a and the first element named b. We will talk more about names when we discuss attributes in general.

Examples:

> x
[1] 3.0 6.0 9.0 10.0 2.2 NA NA 6.7
> y
[1] 1.0 6.0 9.0 2.0 NA 5.1 0.0 -1.0
> x[3]
[1] 9

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```
> x[1:3]

[1] 3 6 9

> x[-2]

[1] 3.0 9.0 10.0 2.2 NA NA 6.7

> x[c(F,T,T,F,F,F,F,F)]

[1] 6.0 9.0

> x[x > y]

[1] 3.0 10.0 NA NA NA 6.7

> x[!is.na(x)]

[1] 3.0 6.0 9.0 10.0 2.2 6.7

> z \leftarrow x[!is.na(x)] # get rid of missing values
```

It is instructive to look at the help file for the subsetting operator "[" (type ?"[") and work out some examples. This is a very useful function that you will be using all the time, but is also very easy to get confused and end up selecting values that you didn't mean to select. Try to always check that you have the right vector by using the length function.

For a simple example of character indexing, let's create a simple named vector.

```
> w ← c(cat=1, dog=3, giraffe=11)
> w['cat']
[1] 1
> w[c('cat','giraffe')]
[1] 1 11
```

2.5 Matrices, Lists and Data Frames

2.5.1 Matrices

A collection of vectors may represent several different variables in your dataset, but is not the most convenient way of handling your data. We can construct matrices by putting together vectors of the same length and the *same mode* using the functions **cbind** and **rbind**. The first one takes its arguments and puts them together as columns of a matrix, while the second one makes them into the rows of a matrix.

```
> x1 \leftarrow c(2,4,6,8,0)
> x2 \leftarrow c(1,3,5,7,9)
> x3 \leftarrow c(3,7,11,15,9)
> cx \leftarrow cbind(x1,x2,x3)
> rx ~ rbind(x1,x2,x3,c(2,6,10,14,8))
> cx
    x1 x2 x3
[1,] 2 1 3
[2,] 4 3 7
[3,] 6 5 11
[4,] 8 7 15
[5,] 0 9 9
>rx
   [,1] [,2] [,3] [,4] [,5]
x1
   2 4 6 8
                          0
```

| x2 | 1 | 3 | 5 | 7 | 9 |
|----|---|---|----|----|---|
| xЗ | 3 | 7 | 11 | 15 | 9 |
| | 2 | 6 | 10 | 14 | 8 |

Notice that that the columns of cx are labeled and so are the rows of rx except for the last one, since the last argument to rbind was not given a name. Another way to create a matrix is to use the function matrix(data,nrow,ncol,...). This function will read data in a stream from the data argument and put it in a nrow × ncol matrix in column order by default. (In fact only one of nrow and ncol is needed if data is of length nrow*ncol). The ... represent other arguments to allow to read the data in row order and give labels to rows and columns.

A useful function to use with matrices is apply. It is invoked by

apply(x,margin,fun,...) where x is a matrix, margin is the dimension over which the function is to be applied (1 for rows, 2 for columns), and fun is the function to be applied to the rows or columns of x.

```
> apply(cx,2,mean)
x1 x2 x3
4 5 9
```

gives us the means of the columns of cx.

Actually apply can be use more generally with multidimensional arrays. Other functions related to matrices are dim, dimnames, is.matrix, ncol, nrow and t. t(x) returns the transpose of x.

Matrices can be indexed in a similar way to vectors. Usually, our purpose is to select a few columns (variables we want to look at) and rows (observations) satisfying a given condition. Since we have two indexes now, we can look at both

The second example above shows another way of selecting two particular columns. Since they are named, we can just list their names in the appropriate place in the indexing bracket. If we don't want to impose any restrictions in a particular dimension, we just leave it blank. Thus, cx[,c("x2","x3")] lists all rows of cx for columns x2 and x3. There are of course, a number of functions to do mathematical operations on matrices: *, %*%, crossprod, and outer which perform element by element multiplication, matrix product, cross products, and outer products, respectively on matrices of the appropriate sizes.

To most efficiently determine which rows of a matrix \mathbf{x} have a column containing an NA, use the expression

is.na(x %*% rep(1,ncol(x)))

To subset the matrix to contain only rows with all non-missing values you can use the Hmisc nomiss function, e.g., nomiss(x).

2.5.2 Lists

Lists are collections of objects of different kinds. The components of a list could be vectors, matrices or other lists and they can have different length and types. An example of a list is the *names* of the rows and columns of a matrix.

The function dimnames is used to name the rows and columns of a matrix and it is required to be a list, so, we used the function list to create it. The arguments to list could be anything, and they can be name just as the rows or columns of a matrix.

```
> list1 <- list(rowmatrix=rx,dimnames(cx),c("a","b","c"))
> list2 \leftarrow list(cx,indexes=1:9)
> list1
$rowmatrix:
   [,1] [,2] [,3] [,4] [,5]
          4
                6
                     8
                          0
     2
x1
x2
      1
           3
                5
                     7
                          9
xЗ
      3
           7
               11
                    15
                          9
x4
      2
           6
              10
                    14
                          8
[[2]]:
[[2]][[1]]:
[1] "1" "2" "3" "4" "5"
[[2]][[2]]:
[1] "x" "y" "z"
[[3]]:
[1] "a" "b" "c"
> list2
[[1]]:
   х у z
1 2 1 3
2 4 3 7
```

```
3 6 5 11
4 8 7 15
5 0 9 9
$indexes:
[1] 1 2 3 4 5 6 7 8 9
```

Components of a list can be selected in one of two ways: the more general method extracts the component by referring to it by its position on the list. list2[[2]] selects the second component of the list list2. If the components are named, we may select them using the expression list\$component or list[['component']]. In the example above, list1\$rowmatrix selects the matrix rx. Ocassionally, you may need the unlisted results. The function unlist serves just such purpose.

There is virtually no limit to what can be stored in a list, including other lists:

```
'Barbour', 'Bibb',...),
+
+
        pop=4273084, capital='Montgomery'),
+
        Alaska=list(counties=c('Aleutians East','Aleutians West',
                             'Anchorage', 'Bethel',...),
+
                   pop=602545, capital='Juneau'),
        ...)
> us$Alabama
                         # Print information for one state
                         # same as us[[1]] or us[['Alabama']]
> us$Alabama$counties
                         # Print counties in Alabama
> us$Alabama$counties[1:5] # Print first 5 counties
> us[c('Alabama','Alaska')] # Print a sub-list containing 2 states
```

Section 2.6.2 provides more information on selecting elements of lists and vectors. You can see that lists provide a natural way to represent hierarchical structures.

In the above example we might as well associate some data with the counties, such as the population:

```
> us \leftarrow list(Alabama=list(counties=c(Autauga=40061,Baldwin=123023,
                                      Barbour=26475,Bibb=18142,...),
+
+
             pop=4273084,capital='Montgomery'),
+
         Alaska=list(counties=c('Aleutians East'=2305,
+
                                 'Aleutians West'=5259,
                                 Anchorage=251336,Bethel=15525,...),
+
+
                     pop=602545, capital='Juneau'),
         ...)
> # Note: need to enclose non-legal S-Plus object names in quotes
> sum(us$Alabama$counties) - us$Alabama$pop
                                                 # should be zero
> us$Alaska$counties['Aleutians East']
                                                 # print one county's population
> us$Alaska$counties['Bethel']
                                                 # print another
> us$Alaska$counties[c('Anchorage','Bethel')] # print two
> Ak \leftarrow us$Alaska
                                                 # subset of list for Alaska
> Ak$counties
                                                 # print Alaska county pops
```

Lists are a very convenient mechanism to summarize in one object all the information related to a particular task. Many functions give as a result a list object. For instance, most modeling functions produce a list whose components are quantities of statistical interest. The function **ols** in the Design library, for example, fits an ordinary least squares model and returns an object of mode list. Among its components are: the model formula, vector of coefficients, summary of missing values, and, optionally, vectors of predicted values, residuals, and the design matrix and response variable values.

2.5.3 Data Frames

Data frames are just a particular kind of list where all its components have the same length. They behave pretty much like matrices in the sense that you can operate on rows and columns and select its elements in the same way, except that the components can be of different type. You may have some columns that are character vectors and other columns that are numeric or logical vectors. Moreover, an entire matrix can be part of a data frame, as long as its columns are of the same length as the other components of the data frame. They are the most similar entity to a SAS dataset that you will find in S, and they are used most frequently in modeling situations, thinking of rows as observations and columns as variables.

There are several ways to create data frames. First, there's the File ... Import dialog. Second, you can read the data into a data frame from an external ASCII or SAS dataset by using the functions read.table or sas.get (to be described later), or construct it from existing objects using the function data.frame.

```
> # Hmisc shorthand for c('id1','id2','id3','id4','id5','id6')
> treat ~ c(rep("Treatment 1",3),rep("Treatment 2",3))
> treat
[1] "Treatment 1" "Treatment 1" "Treatment 1" "Treatment 2" "Treatment 2"
[6] "Treatment 2"
> x \leftarrow c(2.5, 3.5, 3.0, 4.6, 5.5, 5.3)
> df <-- data.frame(treat,x,row.names=obs)
> df
       treat
              x
id1 Treatment 1 2.5
id2 Treatment 1 3.5
id3 Treatment 1 3.0
id4 Treatment 2 4.6
id5 Treatment 2 5.5
id6 Treatment 2 5.3
```

The argument row.names gives names to the rows of the data frame. If provided, its values must be unique. If it is not provided S will try to construct it from the arguments to data.frame. For instance, if one of the arguments is a matrix with a dimnames attribute, it will try to use that. If it can't find any vector to construct the row names, it will simply number them.

The Hmisc naclus and naplot functions are useful for displaying patterns of NAs in data frames in various ways. naclus also returns a vector containing the number of missing variables for each observation. naclus does this using the statements

naclus also returns the mean number of other variables that are missing in observations for which variable *i* is missing, for i = 1, ... See also the builtin **na.pattern** function (Section 2.4.2, but note that **na.pattern** does not work correctly for factor variables).

Data frames may be subsetted using the same notation as matrices (see Section 2.5.1).

2.6 Attributes

We have mentioned certain characteristics of S objects that are typical of that kind of object, and others that are common to all of them. Among the latter ones we can mention the *length* and the *mode* of an object. Length is easy to describe and just counts the number of elements of a vector or matrix, or the number of major components of a list. As a data frame is also a list and its major components are variables, the length of a data frame is the number of variables it contains. The mode refers to the type of object which could be numeric, complex, logical, character (these are called *atomic* objects) or list (which are called *recursive* objects). The functions to find out these characteristics are **length** and **mode** respectively.

The other characteristics that describe an object are referred to as the *attributes* of an object. They include names, dim, dimnames, class, levels, row.names and any other that you may want to create. Corresponding to each of these attributes there is a function to extract them; thus, to know the dim attribute of the matrix cx type dim(cx). To know if a particular observation is in your data frame, we could use the row.names attribute.

```
> row.names(df)[row.names(df)=="id9"]
character(0)
```

The result is a character vector of length zero, meaning that said observation is not in the data frame. Here you could also just print the number of observations with that id using the command sum(row.names(df)=='id9').

In many cases the attribute determines just what kind of and object we have. For instance, a matrix (or more generally, an array) is just a vector with a dim attribute which allow functions such as **apply** to act accordingly. Other functions do not make that distinction and will consider it just a vector.

> length(cx) [1] 15

Attributes can be changed or deleted

```
> \dim(rx) \leftarrow NULL
                      # or attr(rx,'dim') ← NULL
> rx
 [1]
      2 1 3 2 4
                       3
                         7
                             6 6 5 11 10 8 7 15 14 0 9
                                                                  9
                                                                     8
> dim(rx) \leftarrow c(5,4)
> rx
     [,1] [,2] [,3] [,4]
[1,]
        2
              3
                   11
                        14
[2,]
         1
              7
                   10
                         0
[3,]
         З
              6
                   8
                         9
[4,]
         2
              6
                   7
                         9
[5,]
         4
              5
                  15
                         8
```

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rx was a 4×5 matrix. We first made it into a vector by deleting its dim attribute and then made into a 5×4 matrix by assigning a new one. One could also create a new attribute with the function attr.

In this example, the attr function assigns a new attribute called "creation date" to the data frame df, by calling the unix command "date", for example. Next, we listed all the attributes of df using the function attributes. This, not only tells us what attributes df has, but also how they are composed. This might be too much information (specially if you have over a thousand ids in row.names). We can reduce it by typing names(attributes(...)). Notice that the attributes is in general a list with named components, which allows us to use the names function on it.

2.6.1 The Class Attribute and Factor Objects

Notice in the example above, that one of the attributes is called **class**. This is a very special attribute related to the concept of *methods*. When the **class** attribute is present, functions will act in different ways depending on the **class** of the object. **plot** will act in a different way if its arguments have a class of **data.frame**. As usual, the class attribute of an object can be extracted using the function **class**.

```
> class(df)
[1] "data.frame"
```

They can also be unclassified by means of unclass. The result of using unclass is that df will print as a list rather than as a data frame.

> df treat x id1 Treatment 1 2.5 id2 Treatment 1 3.5 id3 Treatment 1 3.0 id4 Treatment 2 4.6 id5 Treatment 2 5.5 id6 Treatment 2 5.3

```
> unclass(df)
$treat:
[1] "Treatment 1" "Treatment 1" "Treatment 2" "Treatment 2"
[6] "Treatment 2"
$treat: Levels:
[1] "Treatment 1" "Treatment 2"
$x:
[1] 2.5 3.5 3.0 4.6 5.5 5.3
attr(, "row.names"):
[1] "id1" "id2" "id3" "id4" "id5" "id6"
attr(, "creation date"):
[1] "Wed Jun 30 10:42:29 EDT 1993"
```

(Note: there is an implicit use of the **print** function when you type **df**). Of particular interest are the objects of class "factor". A *factor* is an object with a discrete set of levels like those that arise from a classification variable. In SAS we could have a variable **x** taking **k** different values, say x_1, \ldots, x_k , with formatted values l_1, \ldots, l_k . In S this will become a *factor* object with internal numeric codes $1, \ldots, k$ and *levels* l_1, \ldots, l_k .

The syntax for the factor function is

```
factor(x,levels,labels,exclude=NA)
```

x is of course the vector to be factored, levels is a vector with the unique set of values of x that you want to keep in the factor, and labels is the corresponding set of optional labels for the values of x. Note the very confusing fact that the labels specified to factor will become the levels attribute of the resulting vector. Those elements of x not matching any element of levels will be considered NA. The exclude argument is a vector of values to be excluded from forming levels. For instance, if x was already a vector of character strings, you may want to set exclude to "" to prevent empty strings from becoming a level.

If you need to use the internal values of x rather than its levels for some reason, the function unclass comes in handy again.

```
> x \leftarrow c(2,2,2,3,3,3)
> 1 \leftarrow c("2","3")
> f \leftarrow factor(x,1)
> x
[1] 2 2 2 3 3 3
> unclass(f)
[1] 1 1 1 2 2 2
attr(, "levels"):
[1] "2" "3"
```

It is not possible to do mathematical transformations of a factor object. The reason is that factors represent categorical variables that may or may not be interval scaled or even ordinal. For example if x and y are factors, it does not make sense to add them.

In summary a factor is a categorical object with a levels attribute, but which is treated internally as having the values 1:length(levels(x)). If no levels argument is provided, the sorted unique values of x are used.

2.6.2 Summary of Basic Object Types

Table 2.1 summarizes some of the types of objects we have discussed. Note that a factor is a special case of a vector, a matrix is a special case of an array, and a data frame is a special case of a list. The table also describes how elements are selected (subscripted) from an object named x. There row and col are vectors of positive, negative, or zero-valued integers, logicals, or character strings (strings are allowed when the pertinent dimension of the object x has a names or dimnames attribute). Zero-valued subscripts are ignored, and negative values denote "get all but the subscripts listed, suppressing their signs." When a subscript is omitted and its place is held by a comma, that means to fetch all elements of the omitted dimension. For lists and data frames, there are 3 methods for selecting elements. The first of these, x[col], results in a new list or data frame containing the elements (usually variables) corresponding to col. The last 2 methods result in individual variables. There colname is the name of *one* of the elements (variables). Below, length is listed as an attribute although it should officially be labeled as a basic property of the object.

| Type | Description | Main Attributes |
|--|---|---|
| vector x[row] | single column of numbers (integer, single, or double precision) or char- acter strings Usually thought of as a <i>variable</i> | length number of elements names (optional) names of ele- ments |
| factor x[row] | categorical variable, with categories coded as integers $1, 2, 3, \ldots$ | length no. elements names (optional) names of elements class 'factor' levels vector of character strings defining labels that correspond to integer codes |
| <pre>matrix x[row,col], x[row,], x[,col]</pre> | rectangular table of numbers or character strings | length number of rows × number of columns dim vector of length 2 containing no. rows, no. columns dimnames list of length 2 contain- ing a vector of row names (or NULL) and a vector of column names (or NULL) |

Table 2.1: Comparison of Some S Objects

| Type | Description | Main Attributes |
|--|---|---|
| list x[col], x\$colname, x[['colname']] | an arbitrary collection of S objects including other lists; can be thought of as a tree; elements do not need to have equal lengths | length number of major elements names names of major elements |
| <pre>data frame x[col], x\$colname, x[['colname']], x[row,col], x[row,], x[,col]</pre> | a rectangular dataset; a list in which all elements have the same number of rows. Each element in the list is a variable, and some of the variables may be matrices | <pre>length number of variables names names of variables class 'data.frame' row.names row (observation)</pre> |

2.7 When to Quote Constants and Object Names

In S you can use single quotes, double quotes, or the Hmisc Cs function (when the symbols being quoted are legal S names) to specify character strings. Here are some general rules about use of quotes.

character constants : Character constants should always be quoted when appearing in S programs. Examples:

object names, general : When a data frame or an object naming a vector or matrix is used as the *input* to a function, do not quote the name. Here are examples:

```
summary(dframe)
attach(dframe)
summary(varname)
mean(varname)
attach(dframe[dframe$sex=='male',])
summary(dframe[,c('age', 'sex')])
```

When giving a function the name of an object to *create*, this name is quoted (see **detach** in the following item).

- variables : These names are generally unquoted except when used to select columns of a data frame, e.g., dframe[,c('age', 'sex')]. If you tried to use dframe[,c(age,sex)], S would combine the values of the age and sex variables and try to use these values as column numbers to retrieve.
- list elements : These are generally not quoted (e.g., when used with \$) unless their names are not legal variable names. In that case use a statement such as objectname[['element name']] or objectname\$'element name'
- removing objects : Do not quote object names given to rm (e.g., rm(age, sex, dframe)). Quote a vector of character constants given to remove, e.g. remove(c('age', 'sex')).
- get and assign : These functions need object names to be quoted, but not the object representing a value for assign to transmit.
- accessing libraries Library names are unquoted when using the library function. They are quoted when using help().

2.8 Function Libraries

S comes with over 2000 functions, organized in the main system areas and in a library of advanced graphics functions called trellis, as well as other libraries. In Windows S-PLUS at least, trellis is automatically available to the user without the need of a library(trellis) command. Other series of functions which are supplied with S are organized into other libraries which must be requested for attachment by the user using the library function. For example, to get access to advanced matrix functions you can type the command library(Matrix). In version 4.5+ you can use the File ... Load Library pull-down menu to issue the library call. For libraries in need of being loaded early in the search list (i.e., those requiring first=T), check the Attach at top of search list box.

Many users have developed add-on libraries of S functions for UNIX, Windows, or both platforms. Frank Harrell has developed two freely available S libraries for UNIX and Windows that are available in the Statlib archive in lib.stat.cmu.edu or from the UVa web page. The Hmisc library ("Harrell Miscellaneous") is described in Section 2.9, and the Design library is described in Chapter 9. Once these libraries are installed⁴, get access to their functions and datasets by typing

```
library(Hmisc, T)  # Reference Hmisc before referencing Design
library(Design,T)  # Design requires Hmisc to work
```

The T (first=T in expanded notation) is needed because Hmisc and Design override a few builtin functions.

Hmisc contains a family of latex functions for converting certain S objects to typeset IAT_EX representation. The output of these functions is a text file containing IAT_EX code. You can also preview typeset IAT_EX files while running S.

 $^{^4}$ These functions are built-in to S-PLUS2000 and later (on Windows only) but they still must be accessed using library() or File ... Load Library

2.9 The Hmisc Library

The Hmisc library contains around 200 miscellaneous functions useful for such things as data analysis, high–level graphics, utility operations, functions for computing sample size and power, translating SAS datasets into S, imputing missing values, advanced table making, variable clustering, character string manipulation, conversion of S objects to $I_{\rm e}T_{\rm E}X$ code, recoding variables, and bootstrap repeated measures analysis. The help categories for Hmisc serve to describe the areas covered by this library:

ANOVA Models Add to Existing Plot Bootstrap Categorical Data **Character Data Operations** Clustering Computations Related to Plotting **Data Directories Data Manipulation** Documentation Grouping Observations **High-Level** Plots Interfaces to Other Languages Linear Algebra Logistic Regression Model Mathematical Operations Matrices and Arrays Methods and Generic Functions Miscellaneous Multivariate Techniques Nonparametric Statistics Overview Power and Sample Size Calculations Predictive Accuracy Printing Probability Distributions and Random Numbers Regression **Repeated Measures Analysis** Robust/Resistant Techniques Sampling Smoothing Operations Statistical Inference Statistical Models Study Design Survival Analysis Utilities

Function Name Purpose _____ abs.error.pred Computes various indexes of predictive accuracy based on absolute errors, for linear models Linear extrapolation approxExtrap aregImpute Multiple imputation based on additive regression, bootstrapping, and predictive mean matching all.is.numeric Check if character strings are legal numerics Nonparametrically estimate transformations for both areg.boot sides of a multiple additive regression, and bootstrap these estimates and R² Optimum sample allocations in 2-sample proportion test ballocation binconf Exact confidence limits for a proportion and more accurate (narrower!) score stat.-based Wilson interval (Rollin Brant, mod. FEH) Bootstrap Kaplan-Meier survival or quantile estimates bootkm Approximate power of 2-sided test for 2 proportions bpower Includes bpower.sim for exact power by simulation bpplot Box-Percentile plot (Jeffrey Banfield, umsfjban@bill.oscs.montana.edu) Sample size requirements for test of 2 proportions bsamsize bystats Statistics on a single variable by levels of >=1 factors bystats2 2-way statistics Calling tree of functions calltree (David Lubinsky, david@hoqax.att.com) character.table Shows numeric equivalents of all latin characters Useful for putting many special chars. in graph titles (Pierre Joyet, pierre.joyet@bluewin.ch) ciapower Power of Cox interaction test cleanup.import More compactly store variables in a data frame, and clean up problem data when e.g. Excel spreadsheet had a nonnumeric value in a numeric column combine.levels Combine infrequent levels of a categorical variable comment Attach a comment attribute to an object: comment(fit) <- 'Used old data'</pre> comment(fit) # prints comment Draws confidence bars on an existing plot using multiple confbar confidence levels distinguished using color or gray scale Print the contents (variables, labels, etc.) of a data frame contents Power of Cox 2-sample test allowing for noncompliance cpower Vector of character strings from list of unquoted names Cs Enhanced importing of comma separated files labels csv.get

A list of functions in Hmisc along with a brief description follows.

| cut2 | Like cut with better endpoint label construction and allows |
|------------------|--|
| datadensity | construction of quantile groups or groups with given n Snapshot graph of distributions of all variables in a data frame. For continuous variables uses scat1d. |
| dataRep | Quantify representation of new observations in a database |
| ddmmmyy | SAS "date7" output format for a chron object |
| deff | Kish design effect and intra-cluster correlation |
| describe | Function to describe different classes of objects. |
| | Invoke by saying describe(object). It calls one of the following: |
| describe.data.f: | rame |
| | Describe all variables in a data frame (generalization of SAS UNIVARIATE) |
| describe.default | t |
| | Describe a variable (generalization of SAS UNIVARIATE) |
| do | Assists with batch analyses |
| dot.chart | Dot chart for one or two classification variables |
| Dotplot | Enhancement of Trellis dotplot allowing for matrix |
| | x-var., auto generation of Key function, superposition |
| drawPlot | Simple mouse-driven drawing program, including a function |
| | for fitting Bezier curves |
| ecdf | Empirical cumulative distribution function plot |
| eip | Edit an object "in-place" (may be dangerous!), e.g. |
| | eip(sqrt) will replace the builtin sqrt function |
| errbar | Plot with error bars (Charles Geyer, U. Chi., mod FEH) |
| event.chart | Plot general event charts (Jack Lee, jjlee@mdanderson.org, |
| | Ken Hess, Joel Dubin; Am Statistician 54:63-70,2000) |
| event.history | Event history chart with time-dependent cov. status |
| | (Joel Dubin, joel.dubin@yale.edu) |
| find.matches | Find matches (with tolerances) between columns of 2 matrices |
| first.word | Find the first word in an S expression (R Heiberger) |
| fit.mult.impute | Fit most regression models over multiple transcan imputations, |
| | compute imputation-adjusted variances and avg. betas |
| format.df | Format a matrix or data frame with much user control |
| | (R Heiberger and FE Harrell) |
| ftupwr | Power of 2-sample binomial test using Fleiss, Tytun, Ury |
| ftuss | Sample size for 2-sample binomial test using " " " " |
| | (Both by Dan Heitjan, dheitjan@biostats.hmc.psu.edu) |
| gbayes | Bayesian posterior and predictive distributions when both |
| | the prior and the likelihood are Gaussian |
| getHdata | Fetch and list datasets on our web site |
| gs.slide | Sets nice defaults for graph sheets for S-Plus 4.0 for |
| | copying graphs into Microsoft applications |
| hdquantile | Harrell-Davis nonparametric quantile estimator with s.e. |
| histbackback | Back-to-back histograms (Pat Burns, Salomon Smith |
| | Barney, London, pburns@dorado.sbi.com) |

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| hist.data.frame | Matrix of histograms for all numeric vars. in data frame Use hist.data.frame(data.frame.name) |
|-----------------|--|
| histSpike | Add high-resolution spike histograms or density estimates |
| haaffd | to an existing plot |
| hoeffd | Hoeffding's D test (omnibus test of independence of X and Y) |
| impute %in% | Impute missing data (generic method) Find out which elements a are in b : a %in% b |
| interaction | More flexible version of builtin function |
| is.present | Tests for non-blank character values or non-NA numeric values |
| james.stein | James-Stein shrinkage estimates of cell means from raw data |
| labcurve | Optimally label a set of curves that have been drawn on |
| | an existing plot, on the basis of gaps between curves. Also position legends automatically at emptiest rectangle. |
| label | Set or fetch a label for an S-object |
| Lag | Lag a vector, padding on the left with NA or '' |
| latex | Convert an S object to LaTeX (R Heiberger & FE Harrell) |
| ldBands | Lan-DeMets bands for group sequential tests |
| list.tree | Pretty-print the structure of any data object |
| Teed | (Alan Zaslavsky, zaslavsk@hcp.med.harvard.edu) |
| Load | Enhanced version of load |
| mask | 8-bit logical representation of a short integer value (Rick Becker) |
| matchCases | Match each case on one continuous variable |
| matxv | Fast matrix * vector, handling intercept(s) and NAs |
| mem | mem() types quick summary of memory used during session |
| mgp.axis | Version of axis() that uses appropriate mgp from |
| | <pre>mgp.axis.labels and gets around bug in axis(2,) that causes it to assume las=1</pre> |
| mgp.axis.labels | |
| | Used by survplot and plot in Design library (and other |
| | functions in the future) so that different spacing |
| | between tick marks and axis tick mark labels may be |
| | specified for x- and y-axes. ps.slide, win.slide, |
| | gs.slide set up nice defaults for mgp.axis.labels. |
| | Otherwise use mgp.axis.labels('default') to set defaults. |
| | Users can set values manually using |
| | mgp.axis.labels(x,y) where x and y are 2nd value of |
| | <pre>par('mgp') to use. Use mgp.axis.labels(type=w) to retrieve values, where w='x', 'y', 'x and y', 'xy',</pre> |
| | to get 3 mgp values (first 3 types) or 2 mgp.axis.labels. |
| minor.tick | Add minor tick marks to an existing plot |
| mtitle | Add outer titles and subtitles to a multiple plot layout |
| mulbar.chart | Multiple bar chart for one or two classification variables |
| %nin% | Opposite of %in% |
| nomiss | Return a matrix after excluding any row with an NA |
| panel.bpplot | Panel function for trellis bwplot - box-percentile plots |
| | |

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| panel.plsmo | Panel function for trellis xyplot - uses plsmo |
|-----------------|---|
| pc1 | Compute first prin. component and get coefficients on original scale of variables |
| plotCorrPrecisi | on Plot precision of estimate of correlation coefficient |
| plsmo | Plot smoothed x vs. y with labeling and exclusion of NAs |
| F | Also allows a grouping variable and plots unsmoothed data |
| popower | Power and sample size calculations for ordinal responses |
| popowor | (two treatments, proportional odds model) |
| prn | prn(expression) does print(expression) but titles the |
| - | output with 'expression'. Do prn(expression,txt) to add |
| | a heading ('txt') before the 'expression' title |
| p.sunflowers | Sunflower plots (Andreas Ruckstuhl, Werner Stahel, |
| F | Martin Maechler, Tim Hesterberg) |
| ps.slide | Set up postcript() using nice defaults for different types |
| P | of graphics media |
| pstamp | Stamp a plot with date in lower right corner (pstamp()) |
| P = = = = = = P | Add ,pwd=T and/or ,time=T to add current directory |
| | name or time |
| | Put additional text for label as first argument, e.g. |
| | pstamp('Figure 1') will draw 'Figure 1 date' |
| putKey | Different way to use key() |
| putKeyEmpty | Put key at most empty part of existing plot |
| rcorr | Pearson or Spearman correlation matrix with pairwise deletion |
| 10011 | of missing data |
| rcorr.cens | Somers' Dyx rank correlation with censored data |
| rcorrp.cens | Assess difference in concordance for paired predictors |
| rcspline.eval | Evaluate restricted cubic spline design matrix |
| rcspline.plot | Plot spline fit with nonparametric smooth and grouped estimates |
| rcspline.restat | e |
| - | Restate restricted cubic spline in unrestricted form, and |
| | create TeX expression to print the fitted function |
| recode | Recodes variables |
| reShape | Reshape a matrix into 3 vectors, reshape serial data |
| rm.boot | Bootstrap spline fit to repeated measurements model, |
| | with simultaneous confidence region - least |
| | squares using spline function in time |
| rMultinom | Generate multinomial random variables with varying prob. |
| samplesize.bin | |
| - | (Rick Chappell, chappell@stat.wisc.edu) |
| sas.get | Convert SAS dataset to S data frame |
| sasxport.get | Enhanced importing of SAS transport dataset in R |
| Save | Enhanced version of save |
| scat1d | Add 1-dimensional scatterplot to an axis of an existing plot |
| | (like bar-codes, FEH/Martin Maechler, |
| | <pre>maechler@stat.math.ethz.ch/Jens Oehlschlaegel-Akiyoshi,</pre> |
| | oehl@psyres-stuttgart.de) |
| | |

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| <pre>score.binary</pre> | Construct a score from a series of binary variables or expressions |
|-------------------------|---|
| sedit | A set of character handling functions written entirely in S. sedit() does much of what the UNIX sed program does. Other functions included are substring.location, substring<-, replace.string.wild, and functions to check if a string is numeric or contains only the digits 0-9 |
| setpdf | Adobe PDF graphics setup for including graphics in books and reports with nice defaults, minimal wasted space |
| setps | Postscript graphics setup for including graphics in books and reports with nice defaults, minimal wasted space Internally uses psfig function by Antonio Possolo (antonio@atc.boeing.com). setps works with Ghostscript to convert .ps to .pdf |
| setTrellis | Set Trellis graphics to use blank conditioning panel strips, line thickness 1 for dot plot reference lines: setTrellis(); 3 optional arguments |
| show.col | Show colors corresponding to col=0,1,,99 |
| show.pch | Show all plotting characters specified by pch=. Just type show.pch() to draw the table on the current device. |
| showPsfrag | Use LaTeX to compile, and dvips and ghostview to display a postscript graphic containing psfrag strings |
| solvet | Version of solve with argument tol passed to qr |
| somers2 | Somers' rank correlation and c-index for binary y |
| spearman | Spearman rank correlation coefficient spearman(x,y) |
| spearman.test | Spearman 1 d.f. and 2 d.f. rank correlation test |
| spearman2 | Spearman multiple d.f. rho ² , adjusted rho ² , Wilcoxon-Kruskal- Wallis test, for multiple predictors |
| spower | Simulate power of 2-sample test for survival under complex conditions Also contains the Gompertz2,Weibull2,Lognorm2 functions. |
| spss.get | Enhanced importing of SPSS files using R's read.spss function |
| src | <pre>src(name) = source("name.s") with memory</pre> |
| stata.get | Enhanced importing of Stata files using R's read.dta function |
| store | store an object permanently (easy interface to assign function) |
| strmatch | Shortest unique identifier match |
| | (Terry Therneau, therneau@mayo.edu) |
| subset | More easily subset a data frame |
| substi | Substitute one var for another when observations NA |
| summarize | Generate a data frame containing stratified summary statistics. Useful for passing to trellis. |
| summary.formula | General table making and plotting functions for summarizing data |
| symbol.freq | X-Y Frequency plot with circles' area prop. to frequency |

| sys | Execute unix() or dos() depending on what's running |
|-----------------|---|
| tex | Enclose a string with the correct syntax for using |
| | with the LaTeX psfrag package, for postscript graphics. |
| transace | ace() packaged for easily automatically transforming all |
| | variables in a matrix |
| transcan | automatic transformation and imputation of NAs for a |
| | series of predictor variables |
| trap.rule | Area under curve defined by arbitrary x and y vectors, |
| | using trapezoidal rule |
| trellis.strip.b | lank |
| | To make the strip titles in trellis more visible, you can |
| | make the backgrounds blank by saying trellis.strip.blank(). |
| | Use before opening the graphics device. |
| t.test.cluster | I |
| uncbind | Form individual variables from a matrix |
| units | Set or fetch "units" attribute - units of measurement for var. |
| upData | Update a data frame (change names, labels, remove vars, etc.) |
| varclus | Graph hierarchical clustering of variables using squared |
| | Pearson or Spearman correlations or Hoeffding D as similarities |
| | Also includes the naclus function for examining similarities in |
| | patterns of missing values across variables. |
| xy.group | Compute mean x vs. function of y by groups of x |
| xYplot | Like trellis xyplot but supports error bars and multiple |
| | response variables that are connected as separate lines |
| win.slide | Setup win.graph or win.printer using nice defaults for |
| | presentations/slides/publications |
| | ar, wtd.quantile, wtd.ecdf, wtd.table, wtd.rank, |
| wtd.loess.noite | r, num.denom.setup |
| | Set of function for obtaining weighted estimates |
| zoom | Zoom in on any graphical display |
| | (Bill Dunlap, bill@statsci.com) |

The web page listed at the front of this document contains several datasets useful in learning about the Hmisc and Design libraries. Two of the data frames are especially useful for learning about logistic modeling with the Design library: titanic and titanic2. Both describe the survival status of individual passengers on the Titanic. The titanic data frame does not contain information from the crew, but it does contain actual ages of half of the passengers.

2.10 Installing Add–on Libraries

For Windows, many of the libraries available in Statlib are transported as compressed (.zip) files. Installation in this case is trivial, as the user merely needs to unzip⁵ the file into the S-PLUS library

⁵Use a recent version of WinZip (from www.winzip.com) or a recent version of unzip that preserves long file names for Windows 95. A good version of unzip is available under Utilities in the Web page listed on the cover of this document. The UVa Web page, under Statistical Computing Tools, has more instructions for installing add-on libraries using WinZip.

area⁶.

Windows S libraries that call Fortran or C routines (as Hmisc and Design do) are so easy to install because the object modules for these routines is stored in a standard format that works on all Windows machines⁷. Therefore the user does not have to have a compiler on her machine. UNIX users install the libraries using a Makefile which invokes compilers as needed. Some users do not have a Fortran 77 or Fortran 90 compiler on their UNIX system; they have to install such a compiler before installing Hmisc or Design. A Fortran-to-C translator produces Fortran code that is too inefficient to be used. Some of the code that needs to be compiled is actually structured Fortran (Ratfor), which needs a Ratfor pre-processor to translate it to Fortran. Users without Ratfor can get pre-processed code already translated to Fortran from FE Harrell⁸.

To install or update the Hmisc or Design library for R, download the appropriate file from http://biostat.mc.vanderbilt.edu/RS (.zip file for Windows; .tar.gz file for Linux/Unix) and store it in a directory for holding temporary files. If using Windows select the appropriate menu to install/update the package from a local file. If using Linux/Unix issue a shell command like R CMD INSTALL /tmp/packagename.tar.gz while logged in as superuser. When Hmisc and Design become part of CRAN, they may be installed like other CRAN packages (e.g., by issuing a command like install.packages('Hmisc') or update.packages('Hmisc') at the R command prompt).

2.11 Accessing Add–On Libraries Automatically

As described in more detail in Section 13.6, you can create a special function in your _Data area that is executed each time S is invoked from your project area. The function is called .First. A common use of .First is to do away with the need to issue a library command each time you invoke S. You can define a .First function once and for all by entering statements such as these in a Commands or Script window.

```
.First ← function() {
    library(Hmisc,T)
    invisible()
}
```

The invisible function prevents the .First function from printing anything when it is invoked.

For R use the command library(Hmisc) instead of library(Hmisc,T). If you create a .First function for R it will be stored in .RData.

Because Hmisc has a variety of basic functions that are useful in routine data analysis and because attaching the Hmisc library carries almost no overhead, it can be a good idea to create such a .First function for each project area ⁹.

⁶E.g., /splus/library as most .zip files for add-on libraries have been created so that during extraction they will be stored in the correct subdirectory of /splus/library.

⁷Similarly, help files are stored in compiled Microsoft Help format, so these also install easily.

⁸But note that S-PLUS comes with a Ratfor pre–processor too.

⁹Hmisc overrides the system subscripting method for factor vectors and date vectors, and it defines functions is.na.dates and is.na.times to check for NAs in date and time vectors. The [.factor redefinition by Hmisc causes by default unused levels to be dropped from the factor vector's levels attribute when the vector is subscripted. This can be overridden by using for example $x \leftarrow x[,drop=F]$ or by specifying a system option as follows: options(drop.factor.levels=F).

Chapter 3

Data in S

3.1 Importing Data

If you are using Windows S-PLUS, most datasets you will need to analyze will be in a format that can be imported easily using the File ... Import dialog. For example, Excel spreadsheets, text (ASCII) files, and data from other popular statistical software can be converted to S-PLUS internal format this way. This method is fast but not all data attributes (e.g., SAS variable labels and value labels) may be imported (see Section 3.2.3). Watch out for non-numeric values in Excel numeric columns, which S-PLUS will import as infinity rather than NA. The Hmisc cleanup.import function will change such values to NA as well as set the storage mode of numeric variables to 'single' or 'integer' depending on whether fractional values are present. This will result in cutting storage in half for numeric variables, as S-PLUS imports these as double precision variables (16 significant digits). cleanup.import also fixes another problem where numeric variables are mistakenly converted to factors. The Hmisc upData function does some of the same functions of cleanup.import in addition to allowing one to change the data frame in many ways (see Section 4.1.5).

The remainder of this chapter deals with commands (functions) for reading and converting data.

3.2 Reading Data into S

3.2.1 Reading Raw Data

The two main functions for reading ASCII datasets into S are scan and read.table. scan is the most versatile of the two, and read.table is easier to use. read.table expects the input data sets to be arranged in tabular form, where the first line may or may not be the variable names. The syntax is

```
> args(read.table)
```

The first argument is a character string reflecting the dataset name; header is set to T if the first line of the file contains the variable names; sep is the separator between fields (by default, any number of blanks); the row.names argument can be an already existing vector of the same length as the number of observations or the name of a variable in the dataset. In either case, it should have no duplicates. col.names is used to give names to variables when header is F and as.is controls which fields are converted to factors. By default, character fields are always made into factor objects. Finally, na.strings can be used whether certain values in character strings should be included as levels of a factor. The result of read.table is a data frame.

The function scan is more complicated and we will only give a sketch here.

The most important arguments here are file and what. The first one is just the name of your dataset, and what is sort of like an INPUT statement. It is a list giving the names and the modes of the data. Example,

In this case, we are reading from the dataset "myfile" the first two columns and naming them pop and city. The O after the equal sign in pop only means that it is going to be read as a numeric variable. Any other number or the expression numeric(O) would have had the same effect. Similarly with the character() expression.

In S-PLUS for Windows you can also read ASCII files using point-and-click methods through the File menu.

3.2.2 Reading S-PLUS Data into R

The best way to transport S-PLUS vectors, matrices, and data frames to other computers or other versions of S-PLUS or to R is to run data.dump() in S-PLUS to create a dumpdata-format (S-PLUS transport format or .sdd file, as described in Section 3.5.2. If using S-PLUS version 5 or later, use the oldStyle=T option to data.dump. Then convert the object to an R object using code such as the following.

You can read binary S objects in _Data or .Data directories and convert them to R objects in some cases using R's read.S function in R's foreign library, if the object was created by S-PLUS versions before version 5 (e.g., conversion of S-PLUS 2000 binary objects usually works). Here is an example:

```
library(foreign)
# Print file _Data/___nonfi to see mapping of renamed files
```

3.2. READING DATA INTO S

```
# to object names
newobj \leftarrow read.S('_Data/__7') # must provide a name to hold result
```

Check the resulting object carefully, because read.S is not foolproof.

3.2.3 Reading SAS Datasets

In many cases, the easiest way to read external files is to read SAS datasets directly. This can be done two ways. First, you can use File ... Import or a standalone database conversion utility such as DBMSCOPY. This approach has the advantages of speed of execution, ease of use, and lack of need of creating temporary ASCII files¹. There are several disadvantages for either fast import method, however: (1) They do not carry SAS variable labels into S. (2) They ignore value labels for categorical variables created using SAS PROC FORMAT. (3) They do not transport SAS special missing values. (4) S variable names constructed from SAS names are in all upper case².

The sas.get function in the Hmisc library for UNIX or Windows is the other approach to convert SAS datasets. sas.get preserves all SAS data attributes, and if categorical variables have customized FORMATs associated with them, sas.get has several options for defining the category labels to S (typically as factor variables).

Long before converting SAS data to S, you should have prepared the SAS dataset so that it would be as useful as possible in SAS. Then **sas.get** can also profit from this setup. Here are the relevant points to consider when creating your SAS dataset:

- 1. Define LABELS on all variables that are not totally self-documenting. The labels should contain mostly lower case letters, as such labels are not only easier to read but they will result in prettier SAS and S output. If you did not take the time to create pretty SAS labels, you can create or override labels after reading the data into S.
- 2. Use the minimum SAS LENGTH that will store each character or numeric variable. For number variables, SAS uses a default of 8 bytes of storage, which is 16 significant digits. Such precision is very seldom needed, and it will result in highly inflated SAS and S datasets. Many SAS variables can be stored as 3 byte floating points, which yields 4 significant digits.
- 3. Define category level definitions using PROC FORMAT, and associate the formats permanently with the appropriate variables.
- 4. Don't store dummy variables and other derived variables (e.g., interaction products) in the permanent SAS dataset, and if you do, don't retrieve them into S as S derives such variables on the fly.

If you do not have nice variable labels or category levels set up in SAS, you can always create them or redefine them in S:

¹The sas.get function has to create temporary ASCII files to do the SAS to S translation.

²This can easily be remedied — see Section 3.4.

The Label function which is documented under the label function will create a text file containing S code defining the existing labels for all the variables in a data frame. You can edit that code, overriding any labels you don't like (including blank ones) and source that file back into S. Call Label using the syntax Label(dataframename, file=). Omit ,file= to write labels to the command window for copying and pasting into an editor window.

Here is the help file for the Windows version of sas.get. The UNIX version does not have the sasout argument, and there are a few other differences. When one or more of the variables you are rescuing from SAS has a PROC FORMAT format associated with it, it is best to use the recode=T option (the default) when invoking sas.get.

sas.get

Convert a SAS Dataset to an S Dataset

sas.get

Converts a SAS dataset into an S data frame. You may choose to extract only a subset of variables or a subset of observations in the SAS dataset. You may have the function automatically convert PROC FORMAT-coded variables to factor objects. The original SAS codes are stored in an attribute called sas.codes and these may be added back to the levels of a factor variable using the code.levels function. Information about special missing values may be captured in an attribute of each variable having special missing values. This attribute is called special.miss, and such variables are given class special.miss. There are print, [], format, and is.special.miss methods for such variables. The chron function is used to set up date, time, and date-time variables. If a date variable represents a partial date (.5 added if month missing, .25 added if day missing, .75 if both), an attribute partial.date is added to the variable, and the variable also becomes a class imputed variable. The describe function uses information about partial dates and special missing values. There is an option to automatically PKUNZIP compressed SAS datasets.

sas.get works by composing and running a SAS job that creates various ASCII files that are read and analyzed by sas.get. You can also run the SAS sas_get macro, which writes the ASCII files for downloading, in a separate step or on another computer, and then tell sas.get to access these files instead of running SAS.

```
sas.get(library, member, variables=<<see below>>, ifs=<<see below>>,
    format.library=library, sasout,
    formats=F, recode=formats, special.miss=F, id=<<see below>>,
    as.is=.5, check.unique.id=T, force.single=F,
    keep.log=T, log.file="_temp_.log", macro=sas.get.macro,
    clean.up=T, sasprog="sas", where, unzip=F)
is.special.miss(x, code)
x[...]
print(x)
format(x)
sas.codes(x)
x ← code.levels(x)
```

ARGUMENTS

library: character string naming the directory in which the the dataset is kept. The default is library=".", indicating that the current directory is to be used.

- member: character string giving the second part of the two part SAS dataset name. (The first part is irrelevant here it is mapped to the directory name.)
 - x: a variable that may have been created by sas.get with special.miss=T or with recode in effect.
- variables: vector of character strings naming the variables in the SAS dataset. The S dataset will contain only those variables from the SAS dataset. To get all of the variables (the default), an empty string may be given. It is a fatal error if any one of the variables is not in the SAS dataset.
 - ifs: a vector of character strings, each containing one SAS "subsetting if" statement. These will be used to extract a subset of the observations in the SAS dataset.
- format.library: The directory containing the file formats.sc2, which contains the definitions of the user defined formats used in this dataset. By default, we look for the formats in the same directory as the data. The user defined formats must be available (so SAS can read the data).
- sasout: If SAS has already run to create the ASCII files needed to complete the creation of the S data frame, specify a vector of 4 character strings containing the names of the files (with full path names if the files are not on the current working directory). The files are in the following order: data dictionary, data, formats, special missing values. This is the same order that the file names are specified to the sas_get macro. For files which were not created and hence not applicable, specify "" as the file name. The presence/absence of formats and special missing data files is used to set the formats and special.miss arguments automatically by sas.get.

sasout may also be a character string of length one, in which case it is assumed to be the name of a .zip file, and sas.get automatically runs the DOS PKUNZIP command to extract the component files to the current working directory. The files that are present in the .zip file must have names "dict", "data", "formats", "specmiss" (although "formats" and "specmiss" do not have to be present). When sas.get is finished, these extracted files are automatically deleted. .zip files are useful for downloading large datasets.

- formats: Set formats to T to examine the format.library for appropriate formats and store them as
 the formats attribute of the returned object (see below). A format is used if it is referred to
 by one or more variables in the dataset, if it contains no ranges of values (i.e., it identifies
 value labels for single values), and if it is a character format or a numeric format that is
 not used just to label missing values. If you set recode to T, 1, or 2, formats defaults to T.
 To fetch the values and labels for variable x in the dataset d you could type: f ←attr(d\$x,
 "format") formats ←attr(d, "formats") formats\$f\$values; formats\$f\$values;
- recode: This parameter defaults to T if formats is T. If it is T, variables that have an appropriate format (see above) are recoded as factor objects, which map the values to the value labels for the format. Alternatively, set recode to 1 to use labels of the form value:label, e.g. 1:good 2:better 3:best. Set recode to 2 to use labels such as good(1) better(2) best(3). Since sas.codes and code.levels add flexibility, the usual choice for recode is T.

- special.miss: For numeric variables, any missing values are stored as NA in S. You can recover special missing values by setting special.miss to T. This will cause the special.miss attribute and the special.miss class to be added to each variable that has at least one special missing value. Suppose that variable y was .E in observation 3 and .G in observation 544. The special.miss attribute for y then has the value list(codes=c("E","G"),obs=c(3,544))) To fetch this information for variable y you would say for example s ←attr(y, "special.miss") s\$codes; s\$obs or use is.special.miss(x) or the print.special.miss method, which will replace NA values for the variable with E or G if they correspond to special missing values. The describe function uses this information in printing a data summary.
 - id: The name of the variable to be used as the row names of the S dataset. The id variable becomes the row.names attribute of a data frame, but the id variable is still retained as a variable in the data frame. You can also specify a vector of variable names as the id parameter. After fetching the data from SAS, all these variables will be converted to character format and concatenated (with a space as a separator) to form a (hopefully) unique ID variable.
 - as.is: SAS character variables are converted to S factor objects if as.is=F or if as.is is a number between 0 and 1 inclusive and the number of unique values of the variable is less than the number of observations (n) times as.is. The default if as.is is .5, so character variables are converted to factors only if they have fewer than n/2 unique values. The primary purpose of this is to keep unique identification variables as character values in the data frame instead of using more space to store both the integer factor codes and the factor labels.
- check.unique.id: If id is specified, the row names are checked for uniqueness if check.unique.id=T.
 If any are duplicated, a warning is printed. Note that if a data frame is being created with
 duplicate row names, statements such as my.data.frame["B23",] will retrieve only the first
 row with a row name of "B23".
- force.single: By default, SAS numeric variables having LENGTHs > 4 are stored as S double precision numerics, which allow for the same precision as a SAS LENGTH 8 variable. Set force.single=T to store every numeric variable in single precision (7 digits of precision). This option is useful when the creator of the SAS dataset has failed to use a LENGTH statement.
- keep.log: logical flag: if F, delete the SAS log file upon completion.
- log.file: the name of the SAS log file.
- macro: the name of an S object in the current search path that contains the text of the SAS macro called by S. The S object is a character vector that can be edited using, for example, sas.get.macro ←editor(sas.get.macro).
- clean.up: logical flag: if T, remove all temporary files when finished. You may want to keep these
 while debugging the SAS macro.
- sasprog: the name of the system command to invoke SAS

- unzip: set to F by default. Set it to T to automatically invoke the DOS PKUNZIP command if member.zip exists, to uncompress the SAS dataset before proceeding. This assumes you have the file permissions to allow uncompressing in place. If the file is already uncompressed, this option is ignored.
- where: by default, a list or data frame which contains all the variables is returned. If you specify where, each individual variable is placed into a separate object (whose name is the name of the variable) using the assign function with the where argument. For example, you can put each variable in its own file in a directory, which in some cases may save memory over attaching a data frame.
- code: a special missing value code (A through Z or underscore) to check against. If code is omitted, is.special.miss will return a T for each observation that has any special missing value.

VALUE

A data frame resembling the SAS dataset. If id was specified, that column of the data frame will be used as the row names of the data frame. Each variable in the data frame or vector in the list will have the attributes label and format containing SAS labels and formats. Underscores in formats are converted to periods. Formats for character variables have \$ placed in front of their names. If formats is T and there are any appropriate format definitions in format.library, the returned object will have attribute formats containing lists named the same as the format names (with periods substituted for underscores and character formats prefixed by \$). Each of these lists has a vector called values and one called labels with the PROC FORMAT; VALUE ... definitions.

SIDE EFFECTS

if a SAS error occurs the SAS log file will be printed under the control of the pager function.

DETAILS

If you specify special.miss=T and there are no special missing values in the data SAS dataset, the SAS step will bomb.

For variables having a PROC FORMAT VALUE format with some of the levels undefined, sas.get will interpret those values as NA if you are using recode.

If you leave the sasprog argument at its default value of "sas", be sure that the SAS executable is in the PATH specified in your autoexec.bat file. Also make sure that you invoke S so that your current project directory is known to be the current working directory. This is best done by creating a shortcut in Windows95, for which the command to execute will be something like drive:\spluswin\cmd\splus.exe HOME=. and the program is flagged to start in drive:\myproject for example. In this way, you will be able to examine the SAS log file easily since it will be placed in drive:\myproject by default.

SAS will create SASWORK and SASUSER directories in what it thinks are the current working directories. To specify where SAS should put these instead, edit the config.sas file or specify a sasprog argument of the following form: sasprog="\sas\sas.exe -saswork c:\saswork -sasuser c:\sasuser".

When sas.get needs to run SAS it is run in iconized form.

The SAS macro **sas_get** uses record lengths of up to 4096 in two places. If you are exporting records that are very long (because of a large number of variables and/or long character variables), you may want to edit these LRECLs to quadruple them, for example.

NOTE

If sasout is not given, you must be able to run SAS on your system.

If you are reading time or date-time variables, you will need to execute the command library(chron) to print those variables or the data frame.

BACKGROUND

The references cited below explain the structure of SAS datasets and how they are stored. See *SAS Language* for a discussion of the "subsetting if" statement.

AUTHORS

Frank Harrell, University of Virginia, Terry Therneau, Mayo Clinic, Bill Dunlap, University of Washington and MathSoft.

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SEE ALSO

data.frame, describe, impute, chron, print.display, label

EXAMPLE

```
> plot(mice$dose, mice$ld50)
> nude.mice ~ sas.get(lib=unix("echo $HOME/saslib"), mem="mice",
   ifs="if strain='nude'")
var=c("dose", "ld50"), ifs="if strain='nude'")
> # Get a dataset from current directory, recode PROC FORMAT; VALUE ...
> # variables into factors with labels of the form "good(1)" "better(2)",
> # get special missing values, recode missing codes .D and .R into new
> # factor levels "Don't know" and "Refused to answer" for variable q1
> attach(d)
> nl \leftarrow length(levels(q1))
> lev \leftarrow c(levels(q1), "Don't know", "Refused")
> q1.new \leftarrow as.integer(q1)
> q1.new[is.special.miss(q1,"D")] ~ nl+1
> q1.new[is.special.miss(q1,"R")] <- nl+2
```

```
> q1.new \leftarrow factor(q1.new, 1:(nl+2), lev)
> # Note: would like to use factor() in place of as.integer ... but
> # factor in this case adds "NA" as a category level
> d \leftarrow sas.get(mem="mydata", recode=T)
> sas.codes(d$x)
                   # for PROC FORMATted variables returns original data codes
> dx \leftarrow code.levels(dx) # or attach(d); x \leftarrow code.levels(x)
> # This makes levels such as "good" "better" "best" into e.g.
> # "1:good" "2:better" "3:best", if the original SAS values were 1,2,3
> # For the following example, suppose that SAS is run on a
> # different machine from the one on which S is run.
> # The sas_get macro is used to create files needed by
> # sas.get (To make a text file containing the sas_get macro
> # run the following S command, for example:
     cat(sas.get.macro, file='/sasmacro/sas_get.sas', sep='\n')
> #
> # Here is the SAS job. This job assumes that you put
> # sas_get.sas in an autocall macro library.
> # libname db '/my/sasdata/area';
> # %sas_get(db.mydata, dict, data, formats, specmiss,
> #
             formats=1, specmiss=1)
>
> # Substitute whatever file names you may want.
> # Next the 4 files are moved to the S machine (using
> # ASCII file transfer mode) and the following S
> # program is run:
id='idvar')
> # If PKZIP is run after sas_get, e.g. "PKZIP port dict data formats"
> # (assuming that specmiss was not used here), use
>
> mydata <-- sas.get(sasout='a:port', id='idvar')
> # which will run PKUNZIP port to unzip a:port.zip, creating the
> # dict, data, and formats files which are interpreted (and leter
> # deleted) by sas.get
```

sas.get calls a SAS macro which produces an ASCII dataset and then uses scan to read it into an S object. If there are errors during the SAS macro processing step, the log file is displayed on the screen (unless quiet=T). This way you can usually know what type of error you have. A common error is that your dataset is in some directory and your formats catalog is in another while omitting the formats.library argument to sas.get (see below). Another error you may find is the message "file such and such not found". On some systems, this condition may occur if your SAS dataset has not been modified in a while and the system compressed it automatically. Set uncompress=T in this case. Also, if you don't have special missing values, do not set special.miss to T.

The sas_get SAS macro specifies the system option NOFMTERR, so if customized formats or format

libraries are not found, SAS will proceed as if the offending variables did not have a format associated with them. This works fine when the undefined formats correspond to variables not requested for retrieval. If however you request a variable having a missing format, you may not know about it until you run describe or other functions.

3.2.4 Handling Date Variables in R

R has a comprehensive way of storing and operating on date, time, and date/time values based on POSIX notation. Type ?DateTimeClasses for details. If you import SAS datasets into R using sas.get, SAS date, time, and date/time variables are automatically converted into R's POSIXct variables.

If you read date/time fields from ASCII text files, the following example shows how to convert into POSIXct variables. Suppose that a comma separated file test.csv contains the following data:

age,date 21,12/31/02 22,01/01/03 23,1/1/02 24,12/1/02 25,12/1/02 26,

The following program can read and recode the data.

```
> mydata
  age
          date
  21 12/31/02
1
2
  22 01/01/03
3
  23
      1/1/02
4
  24 12/1/02
5 25 12/1/02
6 26
> d \leftarrow mydata$date
> d
[1] 12/31/02 01/01/03 1/1/02 12/1/02 12/1/02
Levels: 01/01/03 1/1/02 12/1/02 12/31/02
> d <-- as.POSIXct(strptime(as.character(d),format='%m/%d/%y'))
> # For 4-digit years, use format='%m/%d/%Y'
> # If data were in the format yyyy-mm-dd the conversion would
> # be as simple as d <- as.POSIXct(d)
> d
[1] "2002-12-31 EST" "2003-01-01 EST" "2002-01-01 EST" "2002-12-01 EST"
[5] "2002-12-01 EST" NA
> format(d, '%d%b%Y')
[1] "31Dec2002" "01Jan2003" "01Jan2002" "01Dec2002" "01Dec2002" NA
> # Create a function to make it easy to reformat multiple variables
```

```
as.POSIXct(strptime(as.character(x),format))
+
>
> mydata$date <-- dtrans(mydata$date)
> mydata
 age
          date
1 21 2002-12-31
2 22 2003-01-01
3
 23 2002-01-01
4
 24 2002-12-01
5 25 2002-12-01
6 26
          <NA>
> unclass(mydata$date)
                      # internal values
[1] 1041310800 1041397200 1009861200 1038718800 1038718800
```

3.3 Displaying Metadata

418 observations and 19 variables

The Hmisc contents function displays data about a data frame, including variable labels (if any), units (if any) storage modes, number of NAs, and the number of levels for factor variables. Here is an example.

Maximum # NAs:136

```
> contents(pbc)
```

```
Labels Levels Storage NAs
    bili
                         Serum Bilirubin (mg/dl)
                                                           single
                                                                     0
 albumin
                                  Albumin (gm/dl)
                                                           single
                                                                     0
              Histologic Stage, Ludwig Criteria
                                                           single
                                                                     6
   stage
 protime
                         Prothrombin Time (sec.)
                                                           single
                                                                     2
     sex
                                              Sex
                                                        2 integer
                                                                     0
 fu.days Time to Death or Liver Transplantation
                                                           single
                                                                     0
                                                           single
                                                                     0
     age
                                              Age
 spiders
                                          Spiders
                                                        2 integer 106
                                                        2 integer 106
hepatom
                                     Hepatomagaly
                                                        2 integer 106
 ascites
                                          Ascites
alk.phos
                  Alkaline Phosphatase (U/liter)
                                                           single 106
                                      SGOT (U/ml)
                                                           single 106
    sgot
    chol
                             Cholesterol (mg/dl)
                                                           single 134
    trig
                           Triglycerides (mg/dl)
                                                           single 136
platelet
                       Platelets (per cm<sup>3</sup>/1000)
                                                           single 110
                                        Treatment
                                                        3 integer
    drug
                                                                     0
  status
                                 Follow-up Status
                                                           single
                                                                     0
   edema
                                            Edema
                                                        3 integer
                                                                     0
  copper
                           Urine Copper (ug/day)
                                                           single 108
```

> con <- contents(pbc)</pre>

> print(con, sort='names') # or sort='labels','NAs'

NA

418 observations and 19 variables Maximum # NAs:136

```
Labels Levels Storage NAs
                                               Age
                                                           single
                                                                     0
     age
                                  Albumin (gm/dl)
 albumin
                                                            single
                                                                     0
alk.phos
                  Alkaline Phosphatase (U/liter)
                                                            single 106
                                                        2 integer 106
 ascites
                                          Ascites
. . . .
```

3.4 Adjustments to Variables after Input

Whether raw data or a SAS dataset is used to create a data frame, and whether you used a command or a mouse click to import the data, it is frequently the case that variable names, labels, or value codes need adjustment. These items may be easily changed once and for all or they may be changed every time the data frame is "attached" (see Section 4.1.1). To change variable attributes permanently, the recommended approach is to use the Hmisc upData function (Section 4.1.5). But here are some of the basic methods that are available. For changing individual variables in a list or data frame we rely first on the \$ operator for addressing individual variables in a permanent list of variables. This was introduced in Section 2.5.2. The advantage of making permanent changes in the data frame is that all interactive analyses of that data frame will take advantage of all the new variable names and annotations without prefacing the analysis with statements such as those found below.

In S-PLUS Version 4.x and 2000 it is easy to change variable names by editing column names on a data sheet, but you will have to re-do this every time the source dataset changes and is in need of re-importing. The following method using the edit function has the same disadvantage but it works in all versions of S-PLUS. Suppose that df is the newly created permanent data frame. The names may be edited using

 $names(df) \leftarrow edit(names(df))$

or you can change individual names using for example

names(df)[2] \leftarrow 'Age'

This changed the name of the second variable on the data frame. Here is a trick for changing all the names to lower case:

 $names(df) \leftarrow casefold(names(df))$ # casefold is builtin

Note: When the data are imported from an ASCII file, the best way to specify variable names is to enter them into the "column names" box under the **Options** tab during the file import operation.

To permanently change or define labels for variables, you can use statements such as the following.

label(df\$age) ← 'Age in years'
label(df\$chol) ← 'Cholesterol (mg%)'

To define or change value labels we use the factor function and the levels attribute (if the variable is already a factor). Suppose that one variable, sex, has values 1 and 2 and that we need to define

these as 'female' and 'male', respectively, so that reports and plots will be annotated. Suppose that another variable is already a factor vector, but that we do not like its levels ('a', 'b', 'c'). The following statements will fix both problems.

When a variable is already a factor and you wish to change its levels, you can also use the edit function:

 $levels(v) \leftarrow edit(levels(v))$

Sometimes the input data will contain a factor variable having one or more unused levels. You can delete unused levels from the levels attribute of a variable, say x, by typing $x \leftarrow x[,drop=T]$. If the Hmisc library is in effect you merely have to type $x \leftarrow x[]$ as Hmisc uses a default value of drop=T for its [.factor factor subsetting method.

Other sections show how to define labels and value labels when you only want temporary assignments. This is simpler as you do not need the data frame prefix as in the statements above. You can also **attach** the data frame in search position one to alleviate the need for the \$ prefixing:

```
attach(df, pos=1, use.names=F)
sex ← factor(sex, 1:2, c('female','male'))
levels(treat) ← ...
label(w3) ← 'A-V area'
detach(1, 'df')
```

See Section 4.1.1 for more on this point. See section Section 4.4 for more details about recoding variables, Section 4.1.3 for how to add new variables, and Section 4.1.4 for how to delete variables. Section 4.5 has a review of the many steps one typically goes through to create ready-to-analyze data frames.

See Section 3.1 for more about the cleanup.import function, which can be run on any data frame.

3.5 Writing Out Data

There are generally two instances in which you want to write output to a file. To produce a printed report (which may be enhanced by using some kind of publishing software), or to produce a dataset which may be shared with other users. In the latter case, especially if the other users are not using S-PLUS, the most straightforward way is to use File ... Export or DBMSCOPY or to write an ASCII file. The latter approach can be done with the function write.table.

3.5.1 Writing ASCII files

write.table is very similar to read.table. Its arguments and an example follow.

3.5.2 Transporting S Data

S-PLUS stores objects in an internal binary format that is specific to each hardware platform. Fortunately there is an ASCII transport format that can be used to move objects between any two machines. This format is called *dumpdata* or *transport file* format. You can write *any* S-PLUS object to a transport file using the data.dump function³, and you can read such files using data.restore. These functions also allow you to write or read a single file containing any number of objects. You can use the File ... Export Data or File ... Import Data dialogs to write or read transport files. When you read, all the objects are created or re-created into search position one.

3.5.3 Customized Printing

The basic function for producing customized output is the cat function. When used in conjunction with other functions like paste, round and format, it can print nicely formatted reports. The basic syntax for cat is cat("character string 1",object,"character string 2"). Ex:

```
> cat("The mean of x is",mean(x))
The mean of x is 4.0666666666666667>
```

Two problems are immediately apparent here: one is that mean(x) is producing too many decimals. The other is that cat is not going to a new line after being executed. To go to a new line, the newline character n must be included explicitly. To control the number of digits the functions round or format can be used. round(mean(x),3) will round the output of mean(x) to three significant digits, while format(mean(x)) will print mean(x) with as many digits as the digits options is set.

```
> cat("The mean of x is",round(mean(x),3),"\n")
The mean of x is 4.067
> options()$digits
[1] 7
> options(digits=4)
> cat("The mean of x is",format(mean(x)),"\n")
The mean of x is 4.067
```

The options function controls some of the system options that are assumed by default such as maximum object size, number of digits, width of a printed line, etc. You can see all the options by

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³To make the result backward compatible, specify oldStyle=T to data.dump when running on S-PLUS 5 or 6.

typing options(). The result of this action is a list, that's why we typed options()\$digits to get the value of just the digits option. The effect of format is to coerce objects to become character strings using a common format.

cat prints its arguments in the order in which it encounters them, so, to print something like "value 1 value 2 ... value 10" you would have to type cat("value 1", ... ,"value 10"). The paste function is more efficient for this purpose

> paste("Value",1:10)
[1] "Value 1" "Value 2" "Value 3" "Value 4" "Value 5" "Value 6"
[7] "Value 7" "Value 8" "Value 9" "Value 10"

Using cat in conjunction with paste will give us a nicer output

```
> cat(paste("Value",1:10),fill=8)
Value 1
Value 2
Value 3
Value 4
Value 5
Value 6
Value 7
Value 8
Value 9
Value 10
```

paste returned a character string, using **cat** deleted the quotation marks. The argument **fill** instructed **cat** to put a new line at 8 characters. Other arguments to **cat** include **file** to send the output to a file that you name, **append** to cause **cat** to append any new output to an existing file (or destroy the contents of the file), and **sep** to insert characters between the arguments to **cat** in the output. (**sep=""""** is the default. It can be changed to "" for no spaces).

The print.char.matrix function built-in to S-PLUS is useful for printing hierarchical tables, as it automatically draws boxes separating cells of a table, and each cell can comprise multiple output lines. For R, print.char.matrix is in the Hmisc library.

3.5.4 Sending Output to a File

You can have S send the output of all commands to a file by using the **sink** function. **cat** will only send the results of its output to a file, while **sink** will send the results of every command to a file you name (or a command) until you instruct it not to do so.

```
> sink("myfile") # Send output to file myfile
```

```
> cat("The mean of x is",round(mean(x),3))
```

```
> sink() # Redirect output to the S session
```

3.6 Using the Hmisc Library to Inspect Data

Once the data are read into S, the Hmisc library can be helpful in understanding them as well as checking for "holes" and invalid data. Suppose a data frame named w has been created. Here is a suggested program for taking some initial looks. See Section 4.3.3 for more on the sapply function.

```
# save describe() output
w.des \leftarrow describe(w)
page(w.des, multi=T)
                       # put it in a Window that can linger
win.graph() # open graphics window - openlook(), motif(), X11() for UNIX
            # not needed for S-Plus 4.x or later
# First make a dot chart of the number of NAs for each variable,
# sorting variables so that the worst offender is at the top
m \leftarrow sapply(w, function(x)sum(is.na(x)))
dotplot(sort(m), xlab='NAs')
                               # naplot below does this automatically
                               # gets frequencies of all NA patterns but
na.pattern(m)
                               # treats factor variables as always non-NA
# data and cluster variables according to similarity
                  # of occurrences of NAs
nac
                  # print matrix of pairwise proportions
plot(nac)
                  # cluster NA patterns graphically
naplot(nac)
                  # other displays of patterns of NA
hist.data.frame(w) # matrix of histograms for all non-binary variables
                  # also shows number of NAs
datadensity(w)
                  # make single graph with strip plots (1-dimensional
                  # scatterplots or rug plots) for all variables in w
                  # also consider using builtin plot(w)
ecdf(w)
                  # draw empirical cumulative distributions for all
                  # continuous variables. Also consider using bpplot().
# Now depict how the variables cluster, using squared Spearman rank
# correlation coefficients as similarity measures. varclus uses
# rcorr which does pairwise deletion of NAs
plot(varclus(\sim x1 + x2 + x3 + ..., data=w))
# Assumes variables are named x1, x2, x3, ...
# Use plot(varclus(\sim., data=w)) to analyze all variables
# If any of the variables is missing frequently (say x2), find out what
# predicts its missingness. Use a regression tree
f \leftarrow tree(is.na(x2) ~ x1 + x3, data=w)
# Could have used attach(w) to avoid data= above
plot(f, type='uniform')
text(f)
# Other useful functions for more detailed examinations of the data
# are bwplot, bpplot (box-percentile plots), bwplot with
# panel=panel.bpplot, and symbol.freq (for depicting
# two-way contingency tables).
```

See Section 11.3 for information about the ecdf, datadensity, and bpplot functions, and Section 6.1 for information about symbol.freq. See also the builtin function cdf.compare. And don't forget a wonderful built-in function 'plot.data.frame' that nicely displays continuous variables (using CDFs

turned sideways) and categorical ones (using frequency dot charts). With a high-resolution printer you can see up to 40 variables clearly on a single page. Here is an example.

```
par(mfrow=c(5,8)) # allow up to 40 plots per page
plot(w) # invokes plot.data.frame since w is a data frame
par(mfrow=c(1,1)) # reset to one plot per screen
```

See Section 11.4 for examples of the use of the trellis library instead of datadensity for drawing "strip plots" for depicting data distributions and data densities stratified by other variables.

When you permanently store the result of the describe function (here, in w.des), you can quickly replay it as needed, either by printing it by simply stating its name, or by using page to put it in a new window. If page had already been run with multi=T you merely click on that window's icon to restore it. Note that the page command⁴ causes the pop-up window to remain after you exit from S-PLUS when multi=T. That way you can open the data description whether you are currently in S-PLUS or not. In addition to displaying the w.des object, you can easily display any subset of the variables it describes:

```
w.des[20:30]  # display description of variables 20-30
page(w.des[c(1:10,30:40)])  # page display variables 1-10, 30-40
w.des[c('age','sex')]  # display 2 variables
w.des$age  # display single variable
```

⁴This is true for Windows, and for UNIX if you set your pager to be a window utility such as xless. An excellent pager for Windows is the PFE editor described in Section 1.9. You can set this up by typing options(pager='/pfe/pfe32') or clicking on Options ... General Settings ... Computation, for example. Then by using multiple commands of the form page(object,multi=T) you can have PFE manage all of the pager windows, as by default PFE will add new open files when it is called repeatedly, i.e., it will not invoke an entirely new copy of pfe32.exe. Perhaps an even better pager is an Emacs client. In Windows 95/NT you would set this up by using the command options(pager='gnuclient -q').

Chapter 4

Operating in S

4.1 Reading and Writing Data Frames and Variables

In the introduction we created a subdirectory of your working directory called .Data (or _Data) because this allows for more organized data management, and because this is the default location in which S-PLUS places new data. This way, all the objects that you create for a particular project are available since S-PLUS will search by default in .Data if it exists. However, .Data is not the only directory available to you to store or search for objects. By default, when you start S, a search list is established and a series of directories is accessed sequentially looking for objects or functions. Said list can be modified. The function to display the search list is search(). Its purpose is similar to the PATH command in DOS or UNIX. search() will give us a list of all the directories that S searches looking for functions and data.

- > library(Hmisc, T)
- > library(Design,T)
- > search()
- [1] "_Data"
- [2] "D:\\SPLUSWIN\\library\\Design_Data"
- [3] "D:\\SPLUSWIN\\library\\hmisc_Data"
- [4] "D:\\SPLUSWIN\\splus_Functio"
- [5] "D:\\SPLUSWIN\\stat_Functio"
- [6] "D:\\SPLUSWIN\\s_Functio"
- [7] "D:\\SPLUSWIN\\s_Dataset"
- [8] "D:\\SPLUSWIN\\stat_Dataset"
- [9] "D:\\SPLUSWIN\\splus_Dataset"
- [10] "D:\\SPLUSWIN\\library\\trellis_Data"

The above **search** list contains directories, but you can also attach data frames to the list. When a data frame is in the **search** list, the variables within that data frame are available without using the name of the data frame as a prefix to the variable name.

4.1.1 The attach and detach Functions

To be able to reference objects (data frames, functions, vectors, etc.) that are not in the default **search** path, you can use the **attach** function. The main argument to **attach** is a directory name in single or double quotes or the name of a data frame or list without quotes. As an example, let us attach another directory that contains a variety of S objects. Recall that even in Windows we can specify forward slashes in file and directory names inside of S-PLUS. You can also use a backward slash but it must be doubled, as $\$ is an escape character when inside character strings.

```
> attach('c:/analyses/support/_Data')
```

> search()

```
[1] "_Data"
```

```
[2] "c:/analyses/support/_Data"
```

```
[3] "D:\\SPLUSWIN\\library\\Design\\_Data"
```

```
[4] "D:\\SPLUSWIN\\library\\hmisc\\_Data"
```

- [5] "D:\\SPLUSWIN\\splus_Functio"
- [6] "D:\\SPLUSWIN\\stat_Functio"
- [7] "D:\\SPLUSWIN\\s_Functio"
- [8] "D:\\SPLUSWIN\\s_Dataset"
- [9] "D:\\SPLUSWIN\\stat_Dataset"
- [10] "D:\\SPLUSWIN\\splus_Dataset"
- [11] "D:\\SPLUSWIN\\library\\trellis_Data"

Now list the individual objects in /analyses/support/_Data, which is in search position 2. The objects function (a replacement for an older function, 1s) will do this.

| > objects(2) | | | |
|-----------------|---------------|-----------------|------------|
| [1] ".First" | ".Last.value" | ".Random.seed" | "backward" |
| [5] "combined" | "combphys" | "desc.combined" | "dnrprob" |
| [9] "last.dump" | "mdemoall" | | |

The objects.summary function will provide a more detailed listing. First let's find out how to call it.

```
> args(objects.summary)
function(names. = NULL, what = c("data.class", "storage.mode",
   "extent", "object.size", "dataset.date"), where = 1, frame =
   NULL, pattern = NULL, data.class. = NULL, storage.mode. =
   NULL, mode. = "any", all.classes = F, order. = NULL, reverse
     = F, immediate = T)
> objects.summary(where=2)
             data.class storage.mode
                                           extent object.size
       .First function
                            function
                                               1
                                                          282
  .Last.value describe
                            list
                                               14
                                                        11904
                            integer
 .Random.seed
               numeric
                                              12
                                                           81
                                         6201 x 9
    backward data.frame
                            list
                                                       280180
     combined data frame
                            list
                                      10281 x 150
                                                      7610275
```

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| combphys | data.frame | e li | st | 10281 3 | c 166 | 7025122 |
|---------------|--------------|-------|----|---------|-------|---------|
| desc.combined | describe | e li | st | | 152 | 129733 |
| dnrprob | data.frame | e li | st | 10281 | x 27 | 1283865 |
| last.dump | list | : li: | st | | 3 | 353 |
| mdemoall | data.frame | e li | st | 1757 | x 14 | 136496 |
| | dataset.date | | | | | |
| .First | 96.04.11 | 6:28 | | | | |
| .Last.value | 97.04.11 | 10:18 | | | | |
| .Random.seed | | 0 | | | | |
| backward | 96.04.11 | 6:31 | | | | |
| combined | 97.04.08 | 14:56 | | | | |
| combphys | 97.04.11 | 10:18 | | | | |
| desc.combined | 97.04.08 | 15:01 | | | | |
| dnrprob | 96.09.17 | 17:23 | | | | |
| last.dump | 97.03.06 | 14:07 | | | | |
| mdemoall | 97.04.11 | 10:18 | | | | |

For examples to follow we will use the data frames pbc and prostate. You may obtain these from the Vanderbilt Biostatistics web site under Datasets. The file suffixes are .sdd so they may be easily imported as S-PLUS transport files using File ... Import. Let us suppose these datasets have already been imported into the current project area's Data area. If you are using R or a recent version of the Hmisc library (with wget.exe installed if using Windows) you can easily download and access datasets from the Vanderbilt web site using the Hmisc library's getHdata function.

```
> getHdata(prostate)  # downloads, imports, runs cleanup.import
> find(prostate)
[1] "_Data"
```

First let's examine the variables in **prostate** using the **describe** function in Hmisc. We will first call **describe** on individual variables. As **prostate** has not yet been **attach**ed, we must prefix its variables with **prostate**.

```
> names(prostate)
                                    "status" "age"
[1] "patno" "stage"
                    "rx"
                            "dtime"
                                                    "wt"
                                                            "pf"
                                            "sz"
[9] "hx"
            "sbp"
                    "dbp"
                            "ekg"
                                    "hg"
                                                    "sg"
                                                            "ap"
[17] "bm"
            "sdate"
> describe(prostate$age)
prostate$age : Age in Years
  n missing unique Mean .05 .10 .25 .50 .75 .90 .95
501 1
         41
                71.46 56 60 70 73 76 78
                                            80
lowest : 48 49 50 51 52, highest: 84 85 87 88 89
------
                    _____
> describe(prostate$rx)
prostate$rx : Treatment
  n missing unique
502
         0
               4
placebo (127, 25%), 0.2 mg estrogen (124, 25%), 1.0 mg estrogen (126, 25%)
5.0 mg estrogen (125, 25%)
```

In this example names(prostate) gave us the variables in the data frame and describe(prostate\$age) and describe(prostate\$rx) some basic statistics on a couple of variables. describe recognizes automatically the type of variable (continuous, categorical (factor), or binary) and gives appropriate descriptive statistics (mean and quantiles, frequency table¹, or proportion, respectively), Except for binary variables, the 5 lowest and highest unique values are also given, and for any variable the sample size, number of unique values, and number of missing values is given. When the impute function has been used to impute missing values with "best guesses", describe prints the number of imputed values. When the variable was imported from SAS using sas.get, special missing values were present, and the special.miss option was used, describe will also report the frequency of the various special missing values.

Notice that since **prostate** is a data frame, we are using the \$ notation to refer to its components. This can be rather inconvenient and cumbersome. To make things simpler, we can use the **attach** function to attach the data frame in position one (or two, or whatever) in the search list. By default, **attach** will place objects (which should be data frames or lists) in position 2. The remaining items move down one position.

```
> attach(prostate) # Default placement is search position 2
  > search()
 [1] "_Data"
 [2] "prostate"
 [3] "c:/analyses/support/_Data"
 [4] "D:\\SPLUSWIN\\library\\Design\\_Data"
 [5] "D:\\SPLUSWIN\\library\\hmisc\\_Data"
 [6] "D:\\SPLUSWIN\\splus\\_Functio"
   . . . .
> describe(age)
age : Age in Years
  n missing unique Mean .05 .10 .25 .50 .75 .90 .95
             41
                    71.46 56 60 70 73 76
 501 1
                                              78
                                                  80
lowest : 48 49 50 51 52, highest: 84 85 87 88 89
```

When the data frame (or any other recursive object, e.g., a list) is attached to the search list all its components can be accessed directly. This is the case regardless of the position on the search list. The advantage of using position one is that if you have another version of a variable in another dataframe or directory in the search list, then you can be sure you are operating on the intended version since the search list is accessed sequentially (i.e., we could have used attach(prostate,pos=1,use.names=F)). However, this will use more memory.

If the object is attached in position one, all objects created from now on will be kept in memory and disappear when we quit S-PLUS or detach the object unless we intstruct it to save them (using for example detach(1, 'prostate')). Keep in mind that for large data frames the attach function may take a while to take effect and it will use a lot of memory.

R does not support attaching a data frame in search position one, and at any rate this practice has been found to cause major problems to many programmers, especially those forgetting to detach the data frame upon completion of the modifications to it.

¹If the variable has more than 20 unique values, the frequency table is omitted.

4.1. READING AND WRITING DATA FRAMES AND VARIABLES

Another way to make attach use less memory in S-PLUS is to specify the use.names=F parameter². By default, attaching a data frame causes the row.names attribute of the data frame to be copied to each object within the frame, as that object's name attribute. When for example the row.names represent a subject ID, this can be helpful in identifying observations. But this can result in a doubling of memory usage. It is more efficient to associate names with only the variables whose observations you need to identify, or to just reference the row.names. The example below illustrates these.

```
> attach(titanic, use.names=F)
> record.id ~ row.names(titanic)
> names(pclass) ~ names(age) ~ record.id
> # This isn't so effective here as row.names(titanic) were just
> # record numbers in character form, not passenger names
> # We could have done names(pclass) ~ name
```

The function to take the data frame off the search list is **detach**. It has two arguments, **what** and **save**. **what** is usually a number denoting a postion in the search list and **save** could be a character string with the name of the object where we will store the (possibly) modified data frame.

```
> attach(prostate,pos=1,use.names=F)
> ageg50 ~ age[age>50]
> length(ageg50)
[1] 497
> sqrt.age ~ sqrt(age)
> length(sqrt.age)
[1] 502
> detach(1,save="pros")
Deleted before detaching: ageg50
```

Here we had the data frame prostate attached in position one. We created two new vectors, ageg50 and sqrt.age. Since ageg50 is shorter than the rest of the variables in the data frame it was deleted before detaching and not added to the new data frame pros.

| > names(pros) | | | | | | |
|---------------|------------|---------|------|---------|----------|---------|
| [1] | "patno" | "stage" | "rx" | "dtime" | "status" | "age" |
| [7] | "wt" | "pf" | "hx" | "sbp" | "dbp" | "ekg" |
| [13] | "hg" | "sz" | "sg" | "ap" | "bm" | "sdate" |
| [19] | "sqrt.age" | | | | | |

sqrt.age is a new variable. We could have also said detach(prostate,save=F) which would have deleted sqrt.age before detaching. This form works much faster than trying to save new variables. There is a way to save the value of ageg50 with the dataframe by making it into a *parametrized* dataframe. See Spector's book page 37 for an example. Whether it makes any sense to do this is another matter. Also, we question whether it is useful to create easily derived variables such as sqrt.age, as sqrt(age) may be used in any future S expression where age is analyzed. See Section 4.4.3.

Because attach modifies the search list, its use is sometimes to be discouraged. In R the with function is an excellent substitute in many contexts. This allows one to reference variables inside a data frame using for example

 $^{{}^{2}\}mathsf{R}$ does not have this parameter, and does not put data frame row.names as names attribute of vectors.

```
with(prostate, tapply(age, stage, mean, na.rm=T))
```

Multiple commands may reference variables inside a data frame using for example

```
with(prostate,
   {
    ma ← mean(age, na.rm=T)
    fr ← table(stage)
    print(ma)
})
```

R also allows the analyst to add new variables to a data frame or to recompute existing variables without attach and detach using the transform function.

4.1.2 Subsetting Data Frames

In many cases, one analyzes all of the observations and most of the variables in a data frame. If a subset of the data needs to be analyzed for a small part of the job, one can easily process temporary subsets as in the following examples.

```
plot(age[sex=='male'],height[sex=='male'])
s ← sex=='male'
plot(age[s], height[s]) # equivalent to last example
f ← lrm(death ~ age*height, subset=sex=='male')
```

When you want to subset the observations or variables in a data frame for an entire sequence of operations, it may be better to subset the entire data frame. You can do this by creating a new data frame using

df.males <-- df[df\$sex=='male',]

but more typically by attaching a subset of the data frame. Here are several examples. One of them uses the <code>%nin%</code> operator in the Hmisc library, which returns a vector of T and F values according to whether the corresponding element of the first vector is not contained in the second vector. <code>%nin%</code> is the opposite of the <code>%in%</code> operator in Hmisc.

```
attach(df[,c('age','sex')]) # only make age and sex available - save memory
attach(df[c('age','sex')]) # another way to subset variables using fact
                            # that df is a list in addition to a data frame
attach(df[,Cs(age,sex)])
                           # use the Cs function in Hmisc to save quoting
attach(df[df$sex=='male',]) # get all variables but only for males
                            # need df$sex instead of sex because attach
                            # hasn't taken effect yet
attach(df[1:100,c(1:2,4:7)])# get first 100 rows and variables 1,2,4,5,6,7
attach(df[,-4])
                            # don't get variable number 4
attach(df[,names(df) %nin% c('age','sex')]) # get all but age and sex
attach(df[df$treat %in% c('a','b','d'), names(df) %nin% Cs(age,sex)])
                            # get rows for treatments a,b,d and all but 2 var
attach(df[!(is.na(df$age) | is.na(df$sex)),]) # omit rows containing NAs
attach(df[!is.na(df$age+df$height),])
                                             # shortcut if both vars numeric
```

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After the attach is in effect, referencing any of the included variables will reference the desired subset of rows of the data frame which were attached.

In some ways a more elegant approach is to use the Hmisc subset function which is a copy of the R subset function. The advantages of subset are that variable names do not need prefixing by dataframe\$, and subset provides an elegant notation for subsetting variables by looking up column numbers corresponding to column names given by the user, which allows consecutive variables to keep or drop to be specified. Here are some examples:

```
> # Subset a simple vector
> x1 \leftarrow 1:4
> subset(x1, sex=='male')
[1] 1 3
> # Subset a data frame
> d \leftarrow data.frame(x1=x1, x2=(1:4)/10, x3=(11:14), sex=sex)
> d
 x1 x2 x3
              sex
1 1 0.1 11
             male
2 2 0.2 12 female
3 3 0.3 13 male
4 4 0.4 14 female
> subset(d, sex=='male')
  x1 x2 x3 sex
1 1 0.1 11 male
3 3 0.3 13 male
> subset(d, sex=='male' & x2>0.2)
 x1 x2 x3 sex
3 3 0.3 13 male
> subset(d, x1>1, select=-x1)
  x2 x3
           sex
2 0.2 12 female
3 0.3 13 male
4 0.4 14 female
> subset(d, select=c(x1,sex))
 x1
       sex
  1
      male
1
2 2 female
3 3
      male
4 4 female
> subset(d, x2<0.3, select=x2:sex)</pre>
  x2 x3
           sex
1 0.1 11 male
2 0.2 12 female
```

```
> subset(d, x2<0.3, -(x3:sex))
x1 x2
1 1 0.1
2 2 0.2
> attach(subset(d, sex=='male' & x3==11, x1:x3))
```

4.1.3 Adding Variables to a Data Frame without Attaching

Attaching your data frame in search position one will allow you to add or change any number of variables. There are other ways to add new variables to an existing data frame if you don't want to have the overhead of attaching it. Suppose that we wish to add two variables, x1 and x2, to an existing data frame called df. Here are two approaches:

```
\begin{array}{rll} df\$x1 \ \leftarrow \ pmax(df\$y1, \ df\$y2, \ df\$y3) \\ df\$x2 \ \leftarrow \ (df\$y1 \ + \ df\$y2 \ + \ df\$y3) \ / \ 3 \\ df \ \leftarrow \ data.frame(df, \ x1=pmax(df\$y1, \ df\$y2, \ df\$y3), \\ x2=(df\$y1 \ + \ df\$y2 \ + \ df\$y3)/3) \end{array}
```

4.1.4 Deleting Variables from a Data Frame

Setting a variable to the NULL value will cause it to be deleted permanently from the list³:

```
df$age ← NULL
df[c('age','sex')] ← NULL  # delete 2 variables
df[Cs(age,sex)] ← NULL  # same thing
```

To remove variables that are inside a data frame currently attached in position 1, use statements such as the following.

Do not use rm(varname), remove('varname'), or remove('df\$varname') to remove a variable from a data frame. Use one of the two methods above, or use the object explorer.

4.1.5 A Better Approach to Changing Data Frames: upData

Attaching data frames in search position one turns out to be one of the most confusing and dangerous things to new S-PLUS users. New users tend to forget to detach search position one, and attach a data frame again in search position one, which can at worst corrupt the search list and at best make things very confusing. The Hmisc upData function provides a unified framework for updating a data frame. It accomplishes the following, listed in order in which changes are executed by the function:

- 1. optionally changes names of variables to lower case
- 2. renames variables

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³This is assuming that the data frame is in a directory that is in **search** position 1, e.g., the **_Data** directory. This will not work if **store()** is in effect.

```
3. adds new variables
```

- 4. recomputes existing variables from the original variable and/or from other variables in the data frame
- 5. changes the storage mode of variables to the most efficient mode (as done with cleanup.import) (by default, floating point variables are stored in single precision,⁴ always integer-valued variables are stored as integers)
- 6. drops variables
- 7. adds, changes, and combines levels of factor variables
- 8. adds or changes variable label attributes
- 9. adds or changes variable units (units of measurement) attributes

Here is an example.

```
dat \leftarrow data.frame(a=(1:3)/7, y=c('a', 'b1', 'b2'), z=1:3)
dat2 \leftarrow upData(dat, x=x^2, x=x-5, m=x/10,
             rename=c(a='x'), drop='z',
             labels=list(x='X', y='test'),
             levels=list(y=list(a='a',b=c('b1','b2'))))
# Note that levels b1 and b2 of y are collapsed to 'b'
Input object size: 662 bytes; 3 variables
Renamed variable
                  a to x
Modified variable
                 х
Modified variable x
Added variable
                m
Dropped variable
                 z
New object size: 818 bytes; 3 variables
dat2
        х у
                    m
1 -4.979592 a -0.4979592
2 -4.918367 b -0.4918367
3 -4.816327 b -0.4816326
describe(dat2)
dat2
3 Variables
               3 Observations
_____
х : Х
n missing unique Mean
30
        3
               -4.905
```

 $^{^{4}}$ This is not in R, which has no single precision.

```
-4.816 (1, 33%), -4.918 (1, 33%), -4.980 (1, 33%)
y : test
n missing unique
3
  0
          2
a (1, 33%), b (2, 67%)
                     _____
m
n missing unique
             Mean
30
      3
           -0.4905
-0.4816 (1, 33%), -0.4918 (1, 33%), -0.4980 (1, 33%)
_____
```

A safe approach is to return the result of upData into a new object name, then to check the object (using describe, for example) and to copy it back into the original data frame name. For example,

There are two ways to turn a variable into a factor using upData. First, you can use levels = list(varname = list(...)) as was done above. This is flexible because you can combine levels into "super levels".⁵ Note that new levels are on the left hand side of equal signs, and that these only need to be in quotes if they are not legal S names. The second approach involves recomputing a variable, for example:

4.1.6 assign and store

Up to now we have been storing any new objects that we created permanently in the .Data subdirectory in S-PLUS. Another way to work is to attach the data frame in position one and create temporary objects that we may need with the option to save them later along with the dataframe. If we wanted to save them independently of the dataframe, or you want to put an object in any directory of your choice, the function to use is assign.

```
> args(assign)
function(x, value, frame, where = NULL, ...)
> assign("ageg50",ageg50,where="_Data")  # or .Data in UNIX
> # use assign(...., where='c:/mine/project/_Data') to use another directory
```

This way of working has the advantage to let us create objects temporarily and save only those that we need. That is very useful in an interactive system such as S where one tends to create objects with names like x, y, m, f, etc. The disadvantage is that you have to attach the dataframe in position one, which uses a lot of memory and may slow us down. The **store** function in Hmisc can help you keep your S-PLUS .Data directory from filling up with temporary objects. It can also help in storing objects in permanent locations of your choosing. For the latter purpose **store** works similarly to **assign** except that the order of its arguments is different.

⁵This is done implicitly using the S-PLUS merge.levels function; see its documentation for details.

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```
> args(store)
function(object, name = as.character(substitute(object)), where = ".Data")
```

If you type **store()** with no arguments, then a temporary directory is attached in position one; that way any new objects reside in this temporary area until you quit S-PLUS or decide to store them, either in a dataframe or directly into a subdirectory.

```
> store()
   > attach(prostate)
   > ageg50 \leftarrow age[age>50]
   > sqrt.age \leftarrow sqrt(age)
> search()
 [1] "D:\\SPLUSWIN\\TMP\\file5C9.AD4"
 [2] "_Data"
 [3] "prostate"
 [4] "c:/analyses/support/_Data"
 [5] "D:\\SPLUSWIN\\library\\Design\\_Data"
 . . . .
> objects()
[1] ".Last"
                    ".Last.value" "ageg50"
                                                   "sqrt.age"
   > pros <-- data.frame(prostate,sqrt.age)
   > store(pros) # adds a new variable sqrt.age to the prostate data frame
                  # and store the result in a new permanent data frame pros
   Warning messages:
     "pros" assigned on database 3 but hidden by an object of the same name on
           database 1 in: assign(name, object, where = where, immediate = T)
   > store(ageg50, "age.greater.than.50") # store age50 under the name
                                          # age.greater.than.50, permanently
```

If you have used store(), you can use another function, stores, which is also documented with the store function. stores causes the list of objects (without quotes) to be copied from the temporary directory in search position one to _Data or .Data. Here is an example program that stores two fit objects in the project's _Data directory.

```
df ← sas.get('/my/sasdata','sasmem',recode=T)
store()
fit1 ← lrm(death ~ age*sex)
fit2 ← ols(blood.pressure ~ age*sex)
stores(fit1,fit2) # same as store(fit1);store(fit2)
```

4.2 Managing Project Data in R

R uses a different mechanism from S-PLUS for managing objects that does away with the need to use **store()**. By default, R stores all the objects created in your session in a single file .RData. When running R interactively, R asks whether you want to update .RData to contain newly created objects upon termination of the session. As many of the objects are temporary, it is often best to answer

n to this question and not use the .RData mechanism. It is appropriate however to store some of your newly created data frames and selected other objects (such as regression fit objects that took significant execution time to create) permanently. This can be done using R's **save** function, and if **save**'s **compress** option is used, the resulting file will be stored very compactly. Here is an example session that creates and stores two objects.

```
a ← lm(y ~ x1 + x2)
mydata ← read.csv('/tmp/mydata.csv') # import, creating data frame
save(a, mydata, file='my.rda', compress=TRUE)
# same as save(list=c('a','mydata'), file='my.rda', compress=TRUE)
```

To retrieve the two objects in a future session use

load('my.rda')

When you wish to store objects in .rda files using the same base file name as the name of the object, Hmisc has another way to and objects: the Load and Save functions. :

```
options(LoadPath='../myrdata')  # omit to use current working directory
Save(mydataframe)  # creates ../myrdata/mydataframe.rda
...
Load(mydataframe)  # loads ../myrdata/mydataframe.rda
# creates object mydataframe in .GlobalEnv
```

Save always uses compression, and goes to extra trouble so that the internal name of the saved object will be the name of the argument passed to Save. That way upon Load the newly created object will be referenced by the original object name that was Save'ed. This method has the advantage of having the user define the path for saved objects at the top of the program using options().

4.2.1 Accessing Remote Objects and Different Objects with the Same Names

Ocassionally, we may want to have access to objects stored in some other directory but we don't really want to attach that directory. For example, a fitted model could be stored in some subdirectory and we need to get predicted values from that model using data in the current directory. The get function works very nicely in this case.

Now the model object is available in the temporary directory (under the name z) and we can use it for our needs.

Note: As mentioned above, attaching very big data frames takes a lot of memory and may cause S to slow down significantly unless you have a great deal of RAM installed. It is best to attach only part of the dataframe with the variables and observations you need for each particular problem, if these are a small subset of the entire data.

If you have variables with the same name in the data frame attached in position one and in other directories on the search list as well and you are getting strange or unexpected answers it may be

4.2. MANAGING PROJECT DATA IN R

the case that you are not doing your calculations on the desired variables. For example, suppose that the data frames **prostate** and **pbc** have different versions of the age variable and they are attached in positions three and two respectively. If we mean to get the statistics for **prostate\$age**, **describe(age)** won't do it. This can be problematic if we have to combine data frames from different directories. The **find** function can be helpful here.

```
> attach(prostate)
> attach(pbc)
> search()
[1] ".Data.temp15097"
[2] "pbc"
[3] "prostate"
[4] ".Data"
....
> find(age)
[1] "pbc" "prostate"
```

The masked function is also worth trying. You can have complete control in accessing the desired versions of objects using the get function, or using for example pbc\$age and prostate\$age.

4.2.2 Documenting Data Frames

For long-term projects one frequently needs to document how a data frame came to be, which data were corrected, which data remain suspicious, etc. Besides the obvious method of editing a text document in your project directory, there are at least two ways to have S manage such documentation by linking it to the object.

1. You can attach an attribute to the data frame object. The comment function in the Hmisc library can be used for this. comment attaches or retrieves a comment attribute to the object. You can also invent new attributes. Here are two examples:

See the definition of comment to see how to package the doc attribute more elegantly.

2. You can create a help file for any object you create, so that typing help(objectname) or ?objectname will replay the help file⁶. The help file can contain any text of your choosing, and it should be in a _Help directory underneath the project's _Data directory (.Data/.Help for UNIX).

 $^{^{6}}$ In S-PLUS 3.3 or earlier for Windows this only works if the object name is a legal DOS name with no suffix; otherwise S-PLUS will search for a help file with the name equal to the shortened DOS-version file name, and it won't find it.

4.2.3 Accessing Data in Windows S-PLUS

S-PLUS Windows has an "Object Explorer" that can access data frames (and other objects) and their variables in a way similar to how Windows Explorer traverses directories and opens files. Users can create object explorers that point to one or more data frames in a mixture of _Data directories. Suppose for example that we want to create an object explorer that pointed to all data frames, lists, and matrices in directory c:\projects\one_Data. Here are the required steps. If an object explorer is already open you may want to skip step 1 and use that explorer as a starting point.

- 1. Click on File ... New ... Object Explorer. You'll see a new default object explorer named Object Explorer 1 pop up.
- 2. Left click on SearchPath in the left pane of the object explorer to see the directories currently accessible. Right click on SearchPath and then on Attach Database to add a new area that's not listed. Fill the full path name in the empty box, or use Browse. If you don't want the area put in search position 1 (i.e., you don't want to put all new variables there), select another search position such as 2. Right click in the empty space in the left pain of the Object Explorer. Click on Insert Folder and name it SearchPath. Right click on the new SearchPath folder and select Advanced. Under Interface Objects select SearchPath and click on OK. Right click on the + next to the SearchPath folder and right click on SearchPath under SearchPath. Select Attach Database and specify the directory to add to the search list. Choose search position one for this database if this is where you will be *writing* data.
- 3. Now you will see the above directory listed with a number, the search position, after its name in the right pane of Object Explorer1.
- 4. If you want to specify which kinds of objects in the new area are to be listed by the object explorer, right click while the the cursor is in the open area in the left pane and select Filtering. Now you may see a + in front of the left pane's data.frame entry, and the list of data frames, vectors, and lists on the right pane. Right click on Data and select Advanced. Shift-left-click to add databases to the existing filter list, or regular left click to replace the ones already selected with your new choice. Now Data will show the objects from this new directory.
- 5. Before saving your new object explorer permanently, you may want to modify its name to be more descriptive. While the cursor is in the right pane of your explorer, right click and select Right Pane Click on the Explorer tab and type what you want in the Name and Description fields and click on OK.
- 6. To save this Object Explorer click on File then Save As You can save it in a central _Prefs area or under your project area (by navigating the window which just popped up). For the latter location, click on the ↑ folder to get to the directory and/or disk drive you desire. For this example we get to c:\projects\one. You can override the File name box in the window, to e.g. Project A.sbf. Be sure to include the .sbf at the end of the name.
- 7. When you exit and re-start S-PLUS, you can pop-up your project-specific object explorer by clicking on File. At this point, your object explorer may be on the list at the bottom of the menu so that you can just double click on that. If it's not there, you can click on Open then search for the directory containing it, e.g., c:\projects\one.

4.3. MISCELLANEOUS FUNCTIONS

To use your object explorer, click the + to the left of data.frame (data for object explorer, which will expand this item to list all the data frames present. You can double-click on any of the data frames in this list on the left pane to expand it, i.e., to display its variables and some of their attributes. To display the actual data, double-click on the data frame name in the right pane. This will open a window containing a data sheet.

S-PLUS has a facility for saving and restoring **workspaces**. This is a good way to organize not only databases as was discussed above, but also to link them with reports, graphs, and data sheets. You can set up the workspace so that when it is opened, then active databases not needed by the workspace are detached. Also, when you open a workspace, opened reports and other files are automatically closed.

4.3 Miscellaneous Functions

4.3.1 Functions for Sorting

Table 4.1 displays the functions available for sorting. The obvious choice for sorting a vector

| ÷ | | | |
|---|----------|----------------|------------------------------------|
| | Function | Description | Comments |
| | sort | sort(x) | sorts elements of a vector |
| | order | order(c(x,y,)) | returns the order permutation |
| | rev | rev(x) | reverses the elements of an object |

Table 4.1: Functions for Sorting

is sort. It takes a vector as an argument and returns the vector sorted in ascending order. An optional argument na.last determines if missing values will be discarded, placed at the begining or at the end of the sorted vector (Use na.last=NA, F or T respectively). If it is desired to sort the vector in descending order use rev(sort(x)).

order is more flexible than sort. It returns the order permutation of a vector, that is, its first element is the index corresponding to the smallest element, the second is the index corresponding to the second smallest element, etc. Thus x[order(x)] is equivalent to sort(x). The advantage of order is that it can operate on more than one vector simultaneously. For example order(x,y) will give an order based on x; ties are resolved according to the values of y. To sort a single numeric vector in reverse order you can use -sort(-x) or x[order(-x)]. In the following we sort x alphabetically by state, and within state by descending median.income.

 $\label{eq:state_median_income} \begin{array}{l} \texttt{i} \ \leftarrow \ \texttt{order}(\texttt{state, -median.income}) \\ \texttt{xs} \ \leftarrow \ \texttt{x[i]} \end{array}$

4.3.2 By Processing

You can process observations in groups according to combinations of stratification variables using subscripts, as in the following where we compute the mean **age** stratified by **sex**. Assuming that **sex** is a **factor** object, we can fetch the list of its possible values using the **levels** function.

```
> means 
weans 
single(2) # set aside one position per sex code
> i 
onumber 0
> for(sx in levels(sex)) {
+ i 
onumber i+1
+ s 
onumber sex==sx
+ means[i] 
onumber mean(age[s])
+ }
```

This method is tedious but flexible. We can add logic, for example, to also compute the grand mean.

```
> means \leftarrow single(3)
> i \leftarrow 0
> for(sx in c('ALL',levels(sex))) {
+ i \leftarrow i+1
+ s \leftarrow sex==sx | sx=='ALL'
+ means[i] \leftarrow mean(age[s])
+ }
```

When sx='ALL', s is a vector of all Ts, indicating that all observations should be used in calculating the grand mean.

The above examples are not efficient when typical by processing is to be done. Instead, the function tapply can be used in many situations. In the pbc file, we could get the mean age by stage by doing

The syntax is similar to that of **apply** that we discussed earlier. As we can see, there is no need to sort the data previously. If we wanted to get means by the combination of the levels of two variables we could use

The drop=T argument indicates to drop combinations with no observations in them. Better still, you can easily produce multi-dimensional summaries in array form.

The builtin function by is an excellent way to do by-processing on all the variables in a data frame when the summarization function operates on data frames. Here are some examples.

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```
> by(age, list(Stage=stage), FUN=describe, descript=label(age))
> # descript passed to describe. list(Stage=stage) allows nice labels.
Stage:1
Age
1 Variables 21 Observations
_____
x : Age
 n missing unique Mean .05 .10 .25 .50 .75 .90 .95
21 0 21 46.84 34.60 34.99 38.49 46.35 53.00 59.00 61.99
lowest : 28.88 34.60 34.99 36.00 38.40, highest: 55.57 56.57 59.00 61.99 62.52
_____
Stage:2
Age
1 Variables 92 Observations
_____
x : Age
 n missing unique Mean .05 .10 .25 .50 .75 .90 .95
92 0 87 49.47 33.83 36.58 42.46 49.00 56.39 61.96 63.74
lowest : 30.28 30.57 33.15 33.48 33.62, highest: 63.88 66.41 67.57 68.51 75.01
. . . .
> by(pbc[Cs(age,bili)], list(stage,status), FUN=summary) # or FUN=describe
stage:1
status:0
   age
               bili
Min. :28.9 Min. :0.500
1st Qu.:38.4 1st Qu.:0.600
Median :46.0 Median :0.700
Mean :46.4 Mean :0.805
3rd Qu.:54.3 3rd Qu.:1.000
Max. :62.5 Max. :1.400
_____
stage:2
status:0
age bili
Min. :30.3 Min. : 0.30
1st Qu.:41.8 1st Qu.: 0.60
Median :48.9 Median : 0.70
Mean :48.8 Mean : 1.66
3rd Qu.:56.2 3rd Qu.: 1.40
Max. :75.0 Max. :18.00
_____
stage:3
status:0
. . . .
```

The summary.formula function in Hmisc provides a general way to do by-processing (see Section 6.2). A related function is Hmisc's summarize function, which is designed to compute descriptive statistics stratified by one or more non-continuous variables. summarize creates a data frame useful for processing by other S functions, especially trellis graphics functions, as discussed in Section 11.4.3.

4.3.3 Sending Multiple Variables to Functions Expecting only One

Many of the common S function operate on vectors, e.g., mean, quantile, etc. You can operate on a series of variables or on all the variables in a data frame by looping over the variable names or subscripts, or by using the lapply and sapply functions. The lapply function applies a single function to every element of a list (e.g., every variable in a data frame), and returns a list as the final result, with one list element per variable. For example, let us create a data frame having two variables, and apply the quantile function to each variable:

The **sapply** function formats the results differently. It will produce a vector if the function is single-valued. Here it returns a matrix:

sapply was used in Section 3.6 to plot the number of missing values for all of the variables in a data frame.

When you need to perform a repetitive operation for several variables and you need to be able to access the labels or names of the variables during processing, Hmisc's llist function (documented with the label function) can help. llist tries to use the best available labels for each variable in a list, and it allows you to access these labels using the label function. Here is an example where a series of variables are plotted against a common variable, and each plot is titled with the current variable's label. The sapply (or lapply) methods are preferred if you want to store the result of the function evaluations into a global result.

```
sapply(llist(age, height, pmin(weight,200)),
    function(x) {
        plot(x, blood.pressure)
```

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```
title(label(x))
})
# Equivalent to:
for(x in llist(age, height, pmin(weight,200))) {
   plot(x, blood.pressure)
   title(label(x))
})
```

The S builtin function aggregate is another good method for performing separate analyses of multiple variables in a data frame, with simultaneous stratification on by-variables:

```
> attach(pbc)
                 # so can reference stage without prefix
> aggregate(pbc[Cs(bili,albumin,age)], stage, FUN=mean)
 stage bili albumin age
1
     1 1.36
                3.71 46.8
2
      2 2.45
                3.61 49.5
3
      3 2.83
                3.59 49.0
4
      4 4.43
                3.30 53.8
5
     NA 2.75
                3.32 57.3
  # Same as aggregate(data.frame(bili,albumin,age), stage, FUN=mean)
>
>
  # since we're assuming pbc is attached
```

You must give aggregate a stratification variable. If you want to use aggregate to process multiple variables with no stratification, give it a stratification variable that is constant, e.g., rep(1, length(age)). When there are multiple stratification variables, enclosing them in the Hmisc llist function will cause aggregate to use their names in the data frame it forms. For example, se

> aggregate(data.frame(systolic,diastolic), llist(race,sex), mean)

aggregate can only use FUNs that return a single value although it is able to compute this single value on several response variables. aggregate does not preserve numeric stratification variables (it converts them to factors) so it is not suitable for aggregating some datasets for plotting with xyplot. See p. 238 for a comparison of methods for aggregating data for plotting.

4.3.4 Functions for Data Manipulation and Management

These functions are listed in Table 4.2. seq is a generalization of the ":" operator. It allows us to specify a starting point, an ending point and the distance between them, or alternatively, the length of the resulting vector. We could also specify seq(along=x) which will produce the sequence 1:length(x), even if length(x)=0 (i.e. x is a NULL or numeric(0) vector). duplicated returns a logical vector with T if the index corresponds to a duplicate value, and F if not. unique can be used for example to find the five smallest values of a vector: sort(unique(x))[1:5]. (See the output of describe).

The function match looks up the elements of x in table for each element of x; when it finds a match, it returns the position in table of the match. This can be useful for instance, to join objects, holding the places of non-matching values with missing values.

Comments Description Function seq(a,b,by=z) creates a sequence from **a** to **b** seq with an increment of zin between them duplicated duplicated(x) checks for duplicate values unique(x) returns a vector like **x** unique without repeated values match(x,table) returns the position in table match of the elements of **x** table table(x,y,...) abbreviate abbreviate(x,...) abbreviate text pmatch pmatch(x,table) partial matching expand.grid expand.grid(...) easy way to construct dataframes cut2 an improved version of cut (Hmisc) cut2(x,...)merge(x, y, by, by.x, by.y, ...) merge two data frames merge find.matches(x,y,...) find.matches find closest matches to observations (Hmisc) llist(x,y,...) labeled list of several llist variables (Hmisc) sedit advanced character string manipulation (Hmisc) casefold casefold(strings) change case of vector of character strings or casefold(strings,upper=T) substring substring(strings,start,end) subset char. strings combine infrequent levels (Hmisc) combine.levels combine.levels(x) score.binary recoding (Hmisc) recode recoding (Hmisc) merge.levels merge levels of factor re-shape vectors or matrices (Hmisc) reShape reShape(...)

 $Table \ 4.2: \ Functions \ for \ Data \ Manipulation \ and \ Management$

```
> x \leftarrow 1:10
> y \leftarrow seq(5,15,by=2)
> match(x,y)
 [1] NA NA NA NA 1 NA 2 NA 3 NA
> z \leftarrow cbind(x,y=y[match(x,y)])
> z
       х у
 [1,] 1 NA
 [2,] 2 NA
 [3,] 3 NA
 [4,] 4 NA
 [5,] 5 5
 [6,] 6 NA
 [7,] 7 7
 [8,] 8 NA
 [9,] 9 9
[10,] 10 NA
```

If x and y were dataframes and the matching had been done in their row.names attribute, the result would have been a merged dataframe with NAs for the variables in y where the observation did not match an observation in x. See [3, page 58] for a more detailed example. The merge function is a more general solution to this problem.

abbreviate is especially useful for shortening variable names, row.names, or variable labels, for making output fit on a regular page size. Here are some examples.

The function expand.grid is very useful to produce dataframes with a combination of all levels of specified variables.

```
> z <- expand.grid(age=median(age),rx=levels(rx),bm=c(0,1))
> z
                  rx bm
 age
1 73
             placebo 0
2 73 0.2 mg estrogen 0
3 73 1.0 mg estrogen
                     0
4 73 5.0 mg estrogen
                      0
             placebo
5 73
                      1
6 73 0.2 mg estrogen 1
7 73 1.0 mg estrogen
                     1
8 73 5.0 mg estrogen 1
```

The cut2 function in Hmisc can be used to categorize variables. Unlike cut, the default S function, cut2 returns a factor that is much more useful for analytic purposes. cut2 also has more options and creates better labels for levels of the resulting factor variable.

```
> table(cut2(prostate$age,g=5))
[48,68) [68,72) [72,74) [74,77) [77,89]
96 92 89 123 101
```

The main argument to cut2 is a numeric vector we wish to categorize; it then classifies its argument into g intervals with approximately the same number of observations in them. Instead of g, we could supply the desired cuts via the cuts= argument or the minimum number of observations in each group using the m= argument.

The casefold function was exemplified in Section 3.4.

The substring function is used for pulling apart pieces of character strings. For example, substring('abc',1,2) is 'ab' and substring('abc',2) is 'bc'. substring can be useful for restructuring complex data after input. For example, suppose that dates and times had been stored together in a single character value in a vector x:

> x [1] "98/09/01 00:10" "98/09/01 14:17"

To get the date portion, we substring the first 8 characters of each string and convert it to internal date storage (chron object):

```
> d ← chron(substring(x,1,8), format='y/m/d')
> d
[1] 98/09/01 98/09/01
```

A time variable can be constructed from columns 10-14 of each of these strings. As these times did not include seconds, we paste 0 seconds on to the end of each time using the **paste** function.

Times are stored in hours from midnight. 0.00694 = 10 minutes past midnight, 0.5951 = 14:17:00. Now the dates and times can be recombined into a single date/time **chron** object:

```
> y ← chron(d, tm)
> y
[1] 98/09/01 98/09/01
> print.default(y)
[1] 14123.01 14123.60
```

Dates are stored by default as the number of days from 1Jan1960. If the S chron library is attached, there are more features for printing dates and times.

```
> library(chron)
> tm
[1] 00:10:00 14:17:00
> y
[1] (98/09/01 00:10:00) (98/09/01 14:17:00)
```

Hmisc's combine.levels function is useful for restructuring the levels of a categorical variable, by combining levels have a small proportion of the total frequency. This can be useful for modeling when you want to prevent the construction of a multitude of dummy variables.

See Section 4.4 for examples where the score.binary and recode functions are used. See Sections 6.1 and 4.3.9 for examples of the reShape function.

4.3.5 Merging Data Frames

The merge function is a general function to do one-one, many-one, or many-many joining of two data frames using any number of matching variables. The help file for merge has some excellent examples. Let us consider a common setup where we have a data frame base containing baseline data (one record per subject) and a data frame follow containing multiple records per subject. Both data frames contain a subject identifier variable id. You can use the merge function to do a one-to-many matching merge of the two data frames as in the following example.

```
> base
        ← data.frame(id=c('a','b','c'), age=c(10,20,30))
month=c(1, 2, 1, 2, 3, 2),
                  cholesterol=c(225,226, 320,319,318, 270))
> base
 id age
1 a 10
2 b 20
3
  с
     30
> follow
 id month cholesterol
  a
       1
                 225
1
2
        2
                 226
  а
3
                 320
  b
        1
        2
4
 b
                 319
5 b
        3
                 318
        2
6
 d
                 270
> combined ~ merge(base, follow, by='id', all.x=T)
> # Specify all=T or all.x=T, all.y=T to keep records w/no baseline data
> combined
 id age month cholesterol
1
  a 10
           1
                    225
2
  a
     10
           2
                    226
3
  b
                    320
     20
           1
4
  b
     20
           2
                    319
5
  b 20
           3
                    318
6
  c 30
          NA
                     NA
```

One advantage of this storage format is that it works well with graphics commands in which month is on the x-axis. For example, we can use trellis to plot cholesterol profiles for all subjects with treatment groups in separate panels (if the treatment variable had been stored in the base data frame):

4.3.6 Merging Baseline Data with One–Number Summaries of Follow–up Data

Instead of duplicating baseline data to "spread" it with follow-up data, we often want to summarize the follow-up data into a single number for each subject, and merge this number with the baseline data. In the following example we summarize serial cholesterol measurements using two statistics: the maximum and the mean. We could easily summarize variables besides cholesterol and add them to the chol.summaries data frame below.

```
chol.mean <-- tapply(follow$cholesterol, follow$id, mean, na.rm=T)
chol.summaries \leftarrow data.frame(chol.mean,chol.worst,id=names(chol.mean))
> chol.summaries
 chol.mean chol.worst id
a
    225.5
             226 a
             320 Ъ
    319.0
b
    270.0
             270 d
d
> combined
 id age chol.mean chol.worst
1
 a 10
         225.5
                   226
 b 20
2
         319.0
                   320
3
 c 30
           NA
                   NA
```

4.3.7 Constructing More Complex Summaries of Follow-up Data

Often serial data need summarizations that involve multiple variables simultaneously. In the following example, we have a single date variable and two follow-up measurements (cholest and sys.bp) and we want to save the date and the value of the last non-missing measurements of cholest and sys.bp. The example uses the Hmisc mApply function is a matrix version of tapply.

```
d \leftarrow data.frame(id=c('a', 'a', 'a', 'b', 'b', 'b', 'b'),
                mdate=chron(c('04/02/2001','04/04/2001','05/17/2002',
                   '07/06/2002', '07/07/2002', '08/03/2002', '08/13/2002')),
                cholest =c(210,NA,205, 248,252,251,NA),
                          =c(141,136,NA, 152,NA, 149,151))
                sys.bp
# For R use strptime(c('04/02/2001','''), format='%m/%d/%Y')
d
  id
        mdate cholest sys.bp
  a 04/02/01
                  210
                          141
1
2
  a 04/04/01
                   NA
                          136
3
  a 05/17/02
                  205
                          NA
4
  b 07/06/02
                  248
                          152
5
  b 07/07/02
                  252
                          ΝA
6
  b 08/03/02
                  251
                          149
7 b 08/13/02
                   NA
                          151
```

```
attach(d)
x ← cbind(mdate, cholest, sys.bp)
g \leftarrow function(w) \{
 cholest \leftarrow w[,'cholest']
 \texttt{cholest} \quad \leftarrow \texttt{mean(cholest[mdate==dcholest],na.rm=T)}
 dsys.bp ~ max(mdate[!is.na(sys.bp)],na.rm=T)
 c(dcholest=dcholest,cholest=cholest,dsys.bp=dsys.bp,sys.bp=sys.bp)
}
w \leftarrow mApply(x, id, g)
 dcholest cholest dsys.bp sys.bp
   15477
         205 15069
                        136
а
   15555
           251
               15565
                        151
h
w \leftarrow data.frame(w, id=dimnames(w)[[1]])
# For R: strptime(w$dcholest,format='%Y-%m-%d')
# For S-Plus 6: use dates(w$dcholest)
w
 dcholest cholest dsys.bp sys.bp id
a 05/17/02
         205 04/04/01
                       136 a
ъ 08/03/02
           251 08/13/02
                        151 b
```

The data frame w can be merged (by id) with baseline data as before.

Alternatively, the builtin by function may be used to give useful printed output. However by does not store the result in a useful format.

```
g ← function(w) {
  mdate ← w$mdate
  cholest ← w$cholest
  sys.bp ← w$sys.bp
  dcholest ← max(mdate[!is.na(cholest)],na.rm=T)
  cholest ← mean(cholest[mdate==dcholest],na.rm=T)
  dsys.bp ← max(mdate[!is.na(sys.bp)],na.rm=T)
  dsys.bp ← mean(sys.bp[mdate==dsys.bp],na.rm=T)
  data.frame(dcholest=dcholest,cholest=cholest,dsys.bp=dsys.bp,sys.bp=sys.bp)
}
by(d, d$id, g)
d$id:a
  dcholest cholest dsys.bp sys.bp
1 05/17/02 205 04/04/01 136
```

```
d$id:b
dcholest cholest dsys.bp sys.bp
1 08/03/02 251 08/13/02 151
```

4.3.8 Subsetting a Data Frame by Examining Repeated Measurements

When a data frame consists of data from multiple subjects with repeated records per subject, often the most efficient way to find a single qualifying record per subject and subsetting on qualifying observations is to compute absolute record numbers to retain. Here is an example in R. The record in data frame d that has the earliest date is the one selected. Note that when doing repeated calculations on a variable such as a **Date** variable, calculation time is greatly reduced by first converting the variable to an ordinary numeric vector.

```
d \leftarrow data.frame(id=c('a', 'a', 'a', 'b', 'b', 'b', 'b'),
                  mdate=as.Date(c('04/02/2001','04/04/2001','05/17/2002',
                    <sup>'07/06/2002'</sup>, <sup>'07/07/2002'</sup>, <sup>'08/03/2002'</sup>, <sup>'08/13/2002'</sup>),
         format='%m/%d/%Y'),
                  cholest =c(210,NA,205, 248,252,251,NA),
                  sys.bp =c(141,136,NA, 152,NA, 149,151))
d
  id
           mdate cholest sys.bp
1 a 2001-04-02
                      210
                              141
2
  a 2001-04-04
                       NA
                              136
3
  a 2002-05-17
                      205
                               NA
4
  b 2002-07-06
                      248
                              152
  b 2002-07-07
                      252
                               NA
5
6
  b 2002-08-03
                       251
                              149
7
  b 2002-08-13
                       NA
                              151
numdate \leftarrow as.numeric(d$mdate) # for speed
k \leftarrow with(d, tapply(1:length(numdate), id,
                      function(j) i <- order(numdate[j]); j[i[1]] ))</pre>
k
a b
1 4
d[k,]
  id
           mdate cholest sys.bp
1 a 2001-04-02
                      210
                              141
4
  b 2002-07-06
                      248
                              152
```

4.3.9 Converting Between Matrices and Vectors: Re–shaping Serial Data

Frequently there is a need to convert between matrices and vectors for reformatting how serial measurements are stored. Suppose that a matrix **x** has one row per subject and one column for each time of data collection, with subject IDs and time points documented in **x**'s **dimnames** attribute. To string out this matrix while creating new vectors containing the IDs and times, you can use the following commands.

```
> y \leftarrow as.vector(x) # strung-out vector
> ids \leftarrow dimnames(x)[[1]][row(x)]
> times \leftarrow as.numeric(dimnames(x)[[2]][col(x)])
```

This process is automated with the Hmisc reShape function:

> $w \leftarrow reShape(x)$

This creates a list w with elements rowvar, colvar, and x. rowvar contains the row names of the input matrix (converted to numeric if they are all numeric) corresponding to the current row being represented (variable ids above). colvar contains the corresponding column designations (variable times above), converted to numeric form if possible.

To construct a matrix from an irregular vector of measurements where the subject IDs and time points are defined by ids and times vectors, the following will work.

```
> y
          \leftarrow 1.12
> ids
          \leftarrow c('a', 'b', 'a', 'a', 'b', 'b', 'c', 'c', 'c', 'c', 'd', 'd')
> times \leftarrow c( 1, 1, 3, 5, 4, 5, 1, 3, 4, 5, 3, 5)
          \leftarrow \texttt{ as.factor(ids)}
> idf
> timesf \leftarrow as.factor(times)
          ← matrix(NA,nrow=length(levels(idf)),
> x
                     ncol=length(levels(timesf)),
                     dimnames=list(levels(idf),levels(timesf)))
+
> x[cbind(idf,timesf)] \leftarrow y
> x
   1 3 4 5
  1 3 NA 4
ъ
  2 NA 5 6
c 7 8 9 10
d NA 11 NA 12
```

This is done automatically with the **reShape** function again. Here **reShape** reverses course to reconstruct a matrix because the first argument is now a vector, and the **id** and **colvar** arguments are given.

To create multiple matrices (e.g., one for systolic blood pressure and one for diastolic) and store the re–shaped results in a new data frame, where each matrix column becomes a separate variable, one could do the following:

```
> Sysbp ~ Diasbp ~
+ matrix(NA,nrow=length(levels(idf)),ncol=length(levels(timesf)),
```

```
+ dimnames=list(levels(idf),levels(timesf)))
> dimnames(Sysbp)[[2]] ← paste('sbp',dimnames(Sysbp)[[2]],sep='.')
> dimnames(Diasbp)[[2]] ← paste('dbp',dimnames(Diasbp)[[2]],sep='.')
> age ← c(15, 13, 9, 18)
> # age comes from a non-time-oriented dataframe
> Sysbp[cbind(idf,timesf)] ← sysbp # sysbp is strung-out vector
> Diasbp[cbind(idf,timesf)] ← diasbp
> newdata ← data.frame(age, Sysbp, Diasbp,
+ row.names=levels(idf))
```

The reShape function will create a list containing the multiple matrices:

Here is a similar example using data the **base** and **follow** data frames created above. In this example we merge the re-structured variables with baseline data, forming a new data frame.

```
> idf \leftarrow as.factor(follow$id)
ncol=length(levels(monthf)),
+
               dimnames=list(levels(idf),
+
                paste('chol',levels(monthf),sep='.')))
> serial.chol
 chol.1 chol.2 chol.3
   225
       226
             ΝA
а
   320
       319
            318
b
d
   NA
       270
             NA
> #
                   id=follow$id, colvar=follow$month)
> combined \leftarrow merge(base, follow.t, by='id', all.x=T)
> combined
 id age chol.1 chol.2 chol.3
 a 10
            226
       225
                 NA
1
   20
       320
            319
2
 b
                 318
3
 с
   30
        NA
             NA
                 NA
```

When the first argument to reShape is a vector and the id is a data frame (even with only one variable), reShape will produce a data frame, and the unique groups are identified by combinations of the values of all variables in id. If a data frame constant is specified, the variables in this data frame are assumed to be constant within combinations of id variables (if not, an arbitrary observation in constant will be selected for each group). A row of constant corresponding to the target id combination is then carried along when creating the data frame result. In the following example, we create a data frame, reshaping a long dataset in which groups are formed not just by subject id but by combinations of subject-visit number. We also carry forward a variable that is supposed to be constant within subject-visit number combinations. In this example, it is not

always constant, so an arbitrary visit number will be selected. The R with function is used in place of attach.

```
> w ← data.frame(id=c('a','a','a','a','b','b','b','d','d','d'),
+
              visit=c( 1, 1, 2, 2, 1, 1, 2, 2, 2, 2),
                  k=c('A','A','B','B','C','C','D','E','F','G'),
+
+
                var=c('x','y','x','y','x','y','y','x','y','z'),
               val=1:10)
+
> with(w,
      reShape(val, id=data.frame(id,visit),
+
              constant=data.frame(k), colvar=var))
+
 id visit k x y z
        1 A 1 2 NA
1 a
3
        2 B 3 4 NA
  a
5 b
        1 C 5 6 NA
7 b
        2 D NA 7 NA
8 d
        2 E 8 9 10
```

reShape is also handy for converting predictions for regression models into a table. The expand.grid is frequently used to get predicted values for systematically varying predictors. In the following example there are 3 predictors, of which we allow 2 to vary for getting predicted values. We use reShape to convert the predictions into a matrix, with rows corresponding to the predictor having the most values, and columns corresponding to the other predictor.

```
> d ← expand.grid(x2=0:1, x1=1:100, x3=median(x3))
> pred ← predict(fit, d)
> reShape(pred, id=d$x1, colvar=d$x2) # makes 100 x 2 matrix
```

reShape has a different action when arguments base and reps are specified. It will then reshape a variety of repeated and non-repeated measurements. Serial measurements must have the integers $1, 2, \ldots$ reps at the end of their names. Non-repeated (e.g., baseline) variables are duplicated reps times, and repeated variables are transposed, as shown in the following example.

```
> set.seed(33)
> n ← 4
> w \leftarrow data.frame(age=rnorm(n, 40, 10),
                  sex=sample(c('female', 'male'), n, T),
                  sbp1=rnorm(n, 120, 15),
+
+
                  sbp2=rnorm(n, 120, 15),
+
                  sbp3=rnorm(n, 120, 15),
+
                  dbp1=rnorm(n, 80, 15),
+
                  dbp2=rnorm(n, 80, 15),
+
                  dbp3=rnorm(n, 80, 15), row.names=letters[1:n])
> options(digits=3)
> w
   age
         sex sbp1 sbp2 sbp3 dbp1 dbp2 dbp3
a 35.8 female 126 138 90.2 73.6 60.8 64.4
b 42.5 female 121 133 127.8 86.9 73.8 71.1
c 43.2 male 106 117 138.9 68.6 68.9 83.3
d 50.2 female 127 128 126.8 72.1 66.1 69.7
```

```
> u
 seqno age
              sex
                   sbp dbp
    1 35.8 female 125.8 73.6
а
     2 35.8 female 138.3 60.8
а
     3 35.8 female 90.2 64.4
a
     1 42.5 female 121.4 86.9
b
     2 42.5 female 133.0 73.8
b
b
     3 42.5 female 127.8 71.1
     1 43.2 male 106.1 68.6
С
     2 43.2 male 117.4 68.9
с
     3 43.2 male 138.9 83.3
с
d
     1 50.2 female 126.9 72.1
d
     2 50.2 female 128.3 66.1
d
     3 50.2 female 126.8 69.7
```

If is sometimes the case that multiple variables are represented in "long" form with the name of the variable being stored in a column, and the value of any of the variables stored as a numeric variable value. If in addition to this, a variable is measured on multiple dates within subjects, the situation is a bit more complicated. In the following example, different laboratory measurements are denoted by the values of a character variable lab, and the value of the variable noted in lab is contained in the numeric variable value. The id and date variables can be concatenated together to provide a single unique record identifier, then reshaping can be done on the lab, value pairs.

```
> id ← c('a', 'a', 'a', 'b', 'b', 'b')
> dt \leftarrow c(rep('03/12/1992',3),rep('04/17/1993',2),'05/21/1993')
> date ~ if(.R.) strptime(dt, format='%m/%d/%Y') else chron(dt)
> # .R. is defined by Hmisc; TRUE if running R
> lab \leftarrow c('CBC', 'HA1C', 'ALT', 'CBC', 'HA1C', 'HA1C')
> value \leftarrow 1:6
> data.frame(id, date, lab, value) # show all data (R output follows)
 id
          date lab value
1 a 1992-03-12 CBC
                        1
  a 1992-03-12 HA1C
2
                        2
  a 1992-03-12 ALT
3
                        3
4
  b 1993-04-17 CBC
                        4
5
  b 1993-04-17 HA1C
                        5
6
  b 1993-05-21 HA1C
                        6
> w ← paste(id,date,sep=';')
> d <-- reShape(value, id=w, colvar=lab)
> if(!.R.) d \leftarrow as.data.frame(d)
> d \leftarrow data.frame(d, id=z[[1]],
                 date=if(.R.) strptime(z[[2]], format='%Y-%m-%d') else
+
+
                      as.chron(as.numeric(z[[2]])))
```

> d

ALT CBC HA1C id date a;1992-03-12 3 1 2 a 1992-03-12 b:1993-04-17 4 5 b 1993-04-17 ΝA b;1993-05-21 NA 6 b 1993-05-21 NA

If using S-PLUS 6 and the date variable is a "dates" variable, use dates(z[[2]]) above.

4.3.10 Computing Changes in Serial Observations

One often wants to compute the change in certain variables from one observation to the next. When the observations are aligned into discrete time slots such as month or follow–up visit, it is easiest to reshape serial data into columns and compute differences between columns. In general though, data may not be collected in discrete time slots, and we may want to compute differences between successive observations no matter what time lapses exist. When one of the variables we want to "difference" is the date of the measurements, we can compute time lapses (differences in dates) to compare against the differences in the measurements.

A general approach involves sorting a data frame by subject id and then date within id, and subtracting from each variable of interest the same variable shifted earlier one observation. This will cause the first observation for each subject to be compared with the last observation for the previous subject, but we will have to delete the first observation from each subject anyway, as there is no baseline to subtract from that observation. In the following example we use serial data for three subjects.

```
> d ← data.frame(id=c('a','a','a','b','c','c'),
+
                   visit.date=chron(c('02/03/1997','01/17/1997',
+
                                       '03/01/1997','05/01/1998',
                                       '06/01/1998','05/03/1998')),
+
+
                   height=c(45.2,45,45.8, 52, 56.1, 56),
                   hormone=c(1.3,1.3,1.8, 2.1, 1.9, 1.8))
> # Sort data frame by id, then date
> i
   ← order(d$id, d$visit.date)
> i
[1] 2 1 3 4 6 5
> d \leftarrow d[i,]
> d
  id visit.date height hormone
2
       01/17/97
                   45.0
                            1.3
  a
1
   a
       02/03/97
                   45.2
                            1.3
3
  a
       03/01/97
                   45.8
                            1.8
       05/01/98
4
                   52.0
                            2.1
  b
6
       05/03/98
                   56.0
                            1.8
  с
5
       06/01/98
                   56.1
                            1.9
   с
```

Now we subtract from the current date and height the values from the previous observation. We can shift vectors one observation earlier by putting an NA in front of the vector and ignoring the last element of the vector. This can be done with the following function, which also does preserves attributes of the input variable. This function is one of the undocumented functions in Hmisc.

```
Lag \leftarrow function(x, shift=1) {
  if(is.factor(x)) {
     \texttt{isf}\ \leftarrow\ \texttt{T}
    atr \leftarrow attributes(x)
    atrclass \leftarrow if(length(atr$class)==1) NULL else
       atr$class[atr$class!='factor']
    atr were null \leftarrow NULL
    x \leftarrow as.character(x)
  \} else isf \leftarrow F
  n \leftarrow length(x)
  x \leftarrow x[1:(n-shift)]
  if(!isf) atr \leftarrow attributes(x)
  if(length(atr$label)) atr$label \leftarrow
    paste(atr$label,'lagged',shift,'observations')
  x ← c(rep(if(is.character(x))'' else NA,shift), unclass(x))
  attributes(x) \leftarrow atr
  x
}
```

In what follows the **hormone** level we want to associate with each interval is the value at the start of the interval.

```
> # Put data frame in search position 1 to make permanent changes
> attach(d, pos=1, use.names=F)
> time.lapse <- visit.date - Lag(visit.date)</pre>
> height.change <- height - Lag(height)
> hormone.at.interval.start <- Lag(hormone)
> visit.date \leftarrow height \leftarrow hormone \leftarrow NULL # Remove old variables
> detach(1, 'd2')
> d2
  id time.lapse height.change hormone.at.interval.start
2 a
             NA
                           NA
                                                        NA
1 a
             17
                           0.2
                                                       1.3
3 a
             26
                           0.6
                                                       1.3
4 b
            426
                           6.2
                                                       1.8
6 c
              2
                           4.0
                                                       2.1
5 c
             29
                           0.1
                                                       1.8
```

Now to delete the first record for each subject we must flag these records.

```
> first.id \leftarrow d2$id != Lag(d2$id)
> first.id
[1] TFFTTF
> d2 \leftarrow d2[!first.id,]
> d2
  id time.lapse height.change hormone.at.interval.start
            17
1 a
                          0.2
                                                      1.3
3 a
             26
                           0.6
                                                      1.3
5 c
             29
                           0.1
                                                      1.8
```

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4.4 Recoding Variables and Creating Derived Variables

As discussed in Section 9.4, there are many types of derived variables for which the logical place to state the derivation formula is in a regression model formula. For example, creating dummy variables and storing age² as a separate variable means that you are not using the real power of the S modeling language. Still, there are plenty of occasions for creating or recoding variables. Here is a series of examples showing common ways of creating new variables. See the help file for merge.levels for details about how to change the levels of a factor variable.

```
# compute min(wbc,100000) for each patient
wbc.curtailed \leftarrow pmin(wbc, 100000)
# Still may be better to do this inside a model formula
# Compute a function of height and weight that is different
# for 2 sexes
size 
ifelse(sex=='female',.2*weight^.66/height^.33,
       .25*weight<sup>^</sup>.6/height<sup>^</sup>.3)
# Six ways to combine treatments B and C into one group
# First four assume that treat is a factor object
levels(treat)[levels(treat) %in% c('B', 'C')] ~ 'BC'
# list method causes merge.levels to combine B and C into 'B, C'
levels(treat) \leftarrow list(BC=c('B', 'C')) \# name it BC instead of B, C
# To make multiple merges, do e.g. list(c('B','C'),c('D','E'))
# Group several levels of a categorical variable.
# Leave old variable alone.
# Group levels a b c d into group A, e f g into B, h i into C
y2 \leftarrow y
levels(y2) \leftarrow Cs(A,A,A,B,B,B,C,C) \# or:
levels(y2) \leftarrow list(A=Cs(a,b,c,d), B=Cs(e,f,g), C=Cs(h,i)) # or:
levels(y2) \leftarrow list(Cs(a,b,c,d), Cs(e,f,g), Cs(h,i)) # auto naming
# Categorize a continuous variable (why?)
agecat \leftarrow (age>=30)+(age>=40)+(age>=50)+(age>=60)
# age=41 yields agecat=2. Missing age yields missing agecat
# Could also use agecat \leftarrow cut2(age,c(30,40,50,60))
# Create a 3-category variable coded none, either of two
# conditions is true, or both are true
# First assume that both x1 and x2 are logical or 0-1 variables
z \leftarrow x1 + x2
# Instead, create temporary logical variables from expressions
z \leftarrow (x1="present")+(x2="present")
```

```
z \leftarrow (x1 > 30) + (x2 > 1000)
# Results in x1 <= 30 & x2 <= 1000 : 0
#
            x1 > 30 or x2 > 1000 : 1
#
             x1 > 30 & x2 > 1000 : 2
# Could create a self-documenting variable by:
z2 \leftarrow c('neither', 'either', 'both')[z+1]
# Create a 3-category variable in which the presence of a true for
# the second variable overrides the value of the first variable
z \leftarrow (x1=='present' \& x2=='absent') + 2*(x2=='present')
# Results in x2=='present'& x1=='present' : 2
             x2=='absent' & x1=='present' : 1
#
             x2=='absent' & x1=='absent'
                                           : 0
#
z \leftarrow ifelse(x2=='present', 'x2 present',
            ifelse(x1=='present', 'x1 but not x2', 'neither'))
# Results in x2=='present'
                                           : 'x2 present'
#
             x2=='absent' & x1=='present' : 'x1 but not x2'
             x2=='absent' & x1=='absent' : 'neither'
#
# Create a new categorical variable on the basis of sex and
# whether age>=50. First two ways will produce the same
# coding, all 3 ways produce a good result
g <-- ifelse(sex=='male',
            ifelse(age>=50,'M >= 50','M < 50'),
            ifelse(age>=50,'F >= 50','F < 50'))
g <-- paste(ifelse(sex=='male','M','F'),
           ifelse(age>=50,'>= 50','<50'))
g \leftarrow interaction(sex, age>=50)
```

Recodes to character values can sometimes be done easily by first recoding into integers and then looking up correspondences between the integers and the intended character strings, as shown below.

The second line above applies a sequences of ones and twos as subscripts of the 2 element vector c('domestic','wild'). The result is a vector of character strings of the same length as the vector x, as duplicate ones and twos will result in multiple uses of the character constants. Manipulating levels of a factor variable is easier, implicitly using the merge.levels built-in function.

Recodes from single character string values to numeric or other character values can also be accomplished using a named vector and the subscript operator:

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In the final two lines of output, the animals vector is seen to have a names attribute showing he original values. Note that the name 'guinea pig' had to be enclosed in quotes since it is not a legal S name. We could have done many-to-one recodes by having multiple names for the same character looked-up value. But again, manipulating factor levels is more elegant:

Often it is the case that a large number of categories needs to be recoded into broad groupings. For example, one might wish to categorize medical diagnoses into organ systems or other groupings. It is much easier to do this by constructing a data frame of all individual categories, creating a new character variable to contain the broad category names (initialized to blanks), and to edit the latter (using a data sheet in Windows S-PLUS). In the following example we sort categories by descending frequency of occurrence, initialize categories not used in at least 3 observations to 'other', create a data frame suitable for editing, and then show how to do a table look-up from this new data frame containing category definitions to use them in our main data frame.

The final variable dxgroup is the same length as diagnosis.

Many of the functions in Hmisc and Design use the 'label' attributes of variables. If you are creating printed or graphical output using one of those functions, be sure to define labels to variables you create using Hmisc's label function. You may also want to use Hmisc's units function to define units of measurement. At present, this is only used for survival time objects and for the describe function.

```
map 
(2*diastolic+systolic)/3
label(map) 
'Mean Arterial Blood Pressure'
units(map) 
'mm Hg'
```

4.4.1 The score.binary Function

When you wish to create a new categorical, ordinal, or numeric variable from a series of binary or logical values, the score.binary function in Hmisc may be useful. score.binary summarizes the binary conditions using a hierarchical rule in which the last true value of the series applies, an additive sum is computed, or other user-specified summaries are computed. By default, score.binary uses the first of these three methods is used, i.e., logical true/false variables are examined from left to right, and each observation is classified into the category corresponding to the rightmost true value. The x1,x2 recode example above did this using builtin S language features. Here are the examples from score.binary's help file.

```
# Hierarchical scale, highest of 1:age>70 2:previous.disease
# Here score.binary will return a numeric variable with values 0,1,2
x ← score.binary(age>70, previous.disease, retfactor=F)
# Same as above but return factor variable with levels "none" "age>70"
# "previous.disease":
x ← score.binary(age>70, previous.disease)
# Additive scale with weights 1:age>70 2:previous.disease
x ← score.binary(age>70, previous.disease, fun=sum)
# Additive scale, equal weights
x ← score.binary(age>70, previous.disease, fun=sum, points=c(1,1))
# Same as saying points=1
# Union of variables, to create a new binary variable
x ← score.binary(age>70, previous.disease, fun=any)
```

4.4.2 The recode Function

An undocumented function in Hmisc, recode, may save some time in recoding variable values. recode can handle numeric quantities. When dealing with character or factor vectors it is better to manipulate levels as shown in Section 4.4. Here are some recode examples.

Note that **recode** returned a numeric variable in the last example even though the argument names given to **recode** were '22' and '2'. **recode** checked to see that all of the target values were numeric and that being the case it transformed the result to numeric. Target codes were specified on the left hand side of the equal sign, and when the target codes are legal S names they need not be enclosed in quotes.

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recode can also be called a different way as shown below.

```
> x ← c(1,2,3,3)
> recode(x,1:3,3:1)
[1] 3 2 1 1
> recode(x,1:3,c('a','b','c'))
[1] "a" "b" "c" "c"
> recode(x,1:3,c('cat','dog','rat'))
[1] "cat" "dog" "rat" "rat"
```

recode has some optional arguments. One of them is **none**, which can be used to set the value to return if the original value is not matched by one of the values to recode from.

The match function is also handy for recoding.

```
> x_c('a','b','c','c')
> match(x,c('a','b','c'))
[1] 1 2 3 3
> c('a','b','c')[c(1,2,3,3)]
[1] "a" "b" "c" "c"
```

In the following example, we use a small function **rec** to recode a vector.

```
> rec ~ function(x, from, to) {
+     i ~ match(x, from)
+     to[i]
+ }
> x
> rec(x,c('a','b','c'),c('A','B','C'))
[1] "A" "B" "C" "C"
> rec(x,c('a','b'),c('A','B'))
[1] "A" "B" "" ""
> rec(x,c('a','b','c'),c('ab','ab','c'))
[1] "ab" "ab" "c" "c"
```

4.4.3 Should Derived Variables be Stored Permanently?

If upon leaving S-PLUS you want to be able to re-start S-PLUS and pick up right where you left off, it may be best to store derived variables permanently as separate vectors in **_Data** or in the input data frame:

However, derived variables do take up disk space and they will not automatically be re-derived should you correct one of the original variables used to compute the derived ones. Neither will they be re-derived if you change the derivation formulas. It is thus often better to copy and paste the derivation formulas into the command window from an editor window or to otherwise save the derivation formula for later use. A fancy approach would be to store the derivation formulas as an attribute to the input data frame as shown in the following example.

4.5 Review of Data Frame Creation, Annotation, and Analysis

It is often useful to create, modify, and process datasets in the following order:

- 1. import external data
- 2. make global changes to a data frame (e.g., changing variable names)
- 3. change attributes or values of variables within a data frame
- 4. do analyses involving the whole data frame (without attaching it)
- 5. do analyses of individual variables (after attaching the data frame)

The following program is an example. Here we are processing Rosner's FEV data. First, we do steps that create or manipulate the data frame in its entirety. These are done with _Data in search position one (the S-PLUS default at the start of the session). The cleanup.import function changes numeric variables that are always whole numbers to be stored as integers, the remaining numerics to single precision, strange values from Excel to NAs, and character variables that always contain legal numeric values to numeric variables. cleanup.import typically halves the size of the data frame.

- # The data were imported into data frame FEV to distinguish
- # this name from the variable fev, using File ... Import
- # Source data: Rosner fev.asc (documented in fev.txt)

The renaming of smoking to smoke can also be done using upData. Next we make changes to individual variables within the data frame. When changing more than one or two variables it is most convenient to use upData so that we can omit the data frame and \$ prefix before all the variable names being changed.

```
FEV2 \leftarrow upData(FEV,
               rename=c(smoking='smoke'), # omit if renamed above
               levels=list(sex =list(female=0,male=1),
                           smoke=list('non-current smoker'=0,
                                       'current smoker'=1)),
               units=list(age='years', fev='L', height='inches'),
               labels=list(fev='Forced Expiratory Volume'))
# Check the data frame
page(describe(FEV2), multi=T)
# page makes results go to a new window
# multi=T allows that window to persist while control
# is returned to other windows
# The new data frame is OK. Store it on top of the old FEV and
# then use the graphical user interface to delete FEV2 (click on it
# and hit the Delete key, or type rm(FEV))
FEV \leftarrow FEV2
```

Next, analyses are done that refer to all or almost all variables in the data frame. This is best done without attaching the data frame.

```
summary(FEV)  # basic summary function
plot(FEV)
datadensity(FEV)
hist.data.frame(FEV)
by(FEV, FEV$smoke, summary) # use basic summary with stratification
```

Now, to do detailed analyses involving individual variables, attach the data frame in search position 2.

```
fun=function(y)quantile(y,c(.1,.25,.5,.75,.9)))
plot(s, which=1:5, pch=c(1,2,15,2,1), # pch=c('=','[','o',']','='),
     main='A Discovery', xlab='FEV')
# Use the nonparametric bootstrap to compute a 0.95 confidence
# interval for the population mean fev
smean.cl.boot(fev)
# Use the Statistics ... Compare Samples ... One Sample keys to get
# a normal-theory-based C.I. Then do it more manually. The following
# method assumes that there are no NAs in fev
sd \leftarrow sqrt(var(fev))
xbar \leftarrow mean(fev)
xbar
sd
n \leftarrow length(fev)
qt(.975,n-1)
                 # prints 0.975 critical value of t dist. with n-1 d.f.
xbar + c(-1,1)*sd/sqrt(n)*qt(.975,n-1)
                                           # prints confidence limits
# Fit a linear model
fit \leftarrow lm(fev \sim other variables ...)
```

See Section 3.4 for more details about creating and modifying data frames.

4.6 Dealing with Many Data Frames Simultaneously

Especially when using the sasxport.get function in R to read an entire SAS data library containing dozens of SAS datasets, it is frequently convenient to store the resulting multiple data frames in an S list object. The power of the S language can be used not only to process all datasets in the list in like fashion but to cross-reference variables over datasets and to find inconsistencies in data elements. Here are some examples.

```
> a ~ data.frame(x1=1:3, x2=c('a', 'b', 'c'), x3=2:4)
> a ~ upData(a, labels=c(x1='Label for x1',x3='Label for x3'),
+ units=c(x1='mmHg', x3='minutes'))
> b ~ data.frame(x1=3:5, x4=5:7)
> b ~ upData(b, labels=c(x1='Label for x1'), units=c(x1='cm'))
> d ~ data.frame(x5=1:3, x6=2:4)
> w ~ llist(a,b,d) # llist in Hmisc remembers argument names
> contents(w)
Obs Var Var.NA
a 3 3 0
```

```
b 3 2
          0
d 3 2
         0
> for(u in names(w)) print(describe(w[[u]], descript=u)
а
3 Variables 3 Observations
_____
x1 : Label for x1 [mmHg]
   n missing unique
                 Mean
    3
        0
             3
                    2
1 (1, 33%), 2 (1, 33%), 3 (1, 33%)
_____
x2
   n missing unique
    3 0 3
a (1, 33%), b (1, 33%), c (1, 33%)
_____
x3 : Label for x3 [minutes]
   n missing unique Mean
    3
       0 3
                    3
2 (1, 33%), 3 (1, 33%), 4 (1, 33%)
_____
b
2 Variables 3 Observations
. . .
> datadict \leftarrow
+
  data.frame(dataset=rep(names(w), sapply(w,length)),
         variable=n,
+
         label=unlist(lapply(w, function(x) sapply(x, label))),
+
          units=unlist(lapply(w, function(x) sapply(x, units))),
+
         row.names=NULL)
+
> datadict
 dataset variable
                label
                     units
1
    a
        x1 Label for x1
                     mmHg
2
     a
          x2
3
         x3 Label for x3 minutes
     a
4
         x1 Label for x1 cm
     b
5
    ъ
         x4
6
    d
         x5
7
    d
          x6
```

```
> # print in order of variable names
> datadict[i,]
  dataset variable
                          label
                                  units
1
        a
                x1 Label for x1
                                   mmHg
4
                x1 Label for x1
        b
                                     cm
2
        a
                x2
3
                x3 Label for x3 minutes
        a
5
        b
                x4
6
        d
                x5
7
        d
                x6
> # check for inconsistencies in labels or units (when non-blank)
> chka \leftarrow function(atr) {
>
  w <-- tapply(datadict[[atr]], datadict$variable,
+
               function(x) length(unique(x[x != ""])))
+
   if(any(w > 1))
+
    cat('\nVariables with inconsistent ', atr, ' across datasets:n',
       paste(names(w[w > 1]),collapse=' '),'\n', sep='')
+
+
  invisible()
+ }
> chka('label')
> chka('units')
Variables with inconsistent units across datasets:
x1
```

4.7 Missing Value Imputation using Hmisc

When developing multivariable regression models, the default action of many S functions (and every other system) is to delete an entire row of data when *any* of the variables are missing. In many cases it is a shame to exclude observations missing on X_1 while studying the relationship between X_2 and Y, as this loss of data reduces power and increases variances. Also, deletion of observations containing missing data causes a bias when the data are not missing at random. It is usually better to estimate missing values than to discard valuable data.

When a predictor variable is uncorrelated with all of the other predictors, one can obtain nearly unbiased estimates of regression coefficients (at least in ordinary multiple regression) by replacing missing values with constants. The impute function in Hmisc makes this easy to do. By default, impute will replace missing values with the median non-missing value for continuous variables, and with the most frequent category for categorical (factor) or logical variables. One can specify other statistical functions for use with continuous variables instead of the default fun=median (e.g., fun=mean), or constants or randomly sampled values to insert for numeric or categorical variables. There are methods for printing, subsetting, summarizing, and describing variables having imputed values. There is also a function, is.imputed, that allows easy detection of imputed values. Here are some examples from the impute help file:

```
> age \leftarrow c(1,2,NA,4)
> age.i <- impute(age)
# Could have used impute(age,2.5), impute(age,mean), impute(age,"random")
> age.i
           # Note that print.impute places * after imputed values
 1234
 1 2 2* 4
> summary(age.i)
1 values imputed to 2
Min. 1st Qu. Median Mean 3rd Qu. Max.
    1
        1.75
                   2 2.25
                              2.5
                                     4
> describe(age.i)
age.i
n missing imputed unique Mean
4 0
          1
                   3
                          2.25
1 (1, 25%), 2 (2, 50%), 4 (1, 25%)
> is.imputed(age.i)
[1] F F T F
```

If one developed a model after imputing NAs, it's easy to re-fit the model to see if imputation caused any of the estimated regression shapes to change:

```
> f.noimpute 
update(f, subset=!is.imputed(age))
```

When variables containing NAs are correlated with other variables, it is more accurate to impute these values by predicting them from the other variables. If relationships between variables are monotonic, a tree model may be a convenient approach. In general, customized regression equations may be needed. Hmisc's aregImpute function finds transformations that optimize how each variable is predicted from each other variable using additive semiparametric models (using ace or avas functions). In some cases, one variable can be predicted from another only after a non-monotonic transformation is made on each one. For example, heart rate does not correlate well with blood pressure, but the absolute difference between heart rate and a normal value for heart rate does correlate with the absolute difference between blood pressure and a normal value for blood pressure. aregImpute can find such transformations and base imputations on them. It does imputations, even allowing for missing values in the variables currently being used to predict NAs in the specific variable.

Once aregImpute develops all of the customized imputation models automatically, a special form of the impute function (impute.transcan) can apply the imputations:

But note that the use of fit.mult.impute (see below) is a better approach. Continuous and categorical variables are imputed by aregImpute using predictive mean matching.

It is well known that ignoring the fact that imputations were done will bias standard error estimates downward. Estimated standard errors can be corrected using multiple imputation, but it is also easy to use the bootstrap. The bootstrap can also adjust for other sources of variation such as stepwise variable selection or estimating transformations of the response variabel. Bootstrapping is not usually practical when using aregImpute because aregImpute often runs too slowly to be called inside a bootstrap loop. Here is an example when imputations are done using a constant. See Section 4.8 for another bootstrap example.

```
> store()
           # don't keep any objects from this session
> # Generate data with no missing values
> n ← 200
> set.seed(231)
> x1 \leftarrow rnorm(n)
> x2 \leftarrow sample(0:1, n, replace=T)
> y \leftarrow x1 + 2*x2 + rnorm(n)/3
# Make 40 of the x1 values missing at random
> x1[sample(1:length(x1), 40)] \leftarrow NA
> describe(x1)
x1
   n missing unique
                      Mean
                                  .05
                                           .10
                                                     .25
                                                               .50
 160 40
           160
                     0.02925 -1.82198 -1.40211 -0.62995 0.05152
      .75
             . 90
                        . 95
  0.83800 1.27483 1.65581
> # Impute missing x1s using the median of non-missing x1s
> x1i \leftarrow impute(x1)
> # Fit linear regression model using Design library's ols function
> f \leftarrow ols(y \sim x1i + x2, x=T, y=T)
> # Print standard errors that were computed using the standard formula
> sqrt(diag(f$var))
[1] 0.05802961 0.04385920 0.08295235
> # Compute bootstrap estimates of standard errors not corrected for imputation
> B ← 300
> sqrt(diag(bootcov(f, B=300, pr=T)$var))
[1] 0.05441155 0.02582960 0.08077475
> # Note that these standard errors are unconditional estimates whereas
> # Standard formulas use variables conditional on covariable values
> # Now correct for imputation. The following calculations are the same
> # used by bootcov except that imputation is done inside the bootstrap loop
> betas ~ matrix(NA, nrow=B, ncol=3)
> for(i in 1:B) {
    cat(i,'')
    j \leftarrow sample(1:n, n, rep=T) \# bootstrap sample
   x1b \leftarrow x1[j]
    x1bi \leftarrow impute(x1b)
+
```

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[1] 0.06436752 0.02908877 0.08260003

```
+ x2b ← x2[j]
+ yb ← y[j]
+ cof ← lm.fit.qr(cbind(1,x1bi,x2b), yb)$coefficients
+ # lm.fit.qr is used internally by ols and lm. Use it here for
+ # raw speed. Even faster- use undocumented Hmisc function:
+ # cof ← lm.fit.qr.bare(cbind(x1bi,x2b), yb)$coefficients
+ betas[i,] ← cof
+ }
> sqrt(diag(var(betas)))
```

We see that when correcting for imputation the standard error of the intercept and of the regression coefficient for x1 increased the most.

Caution: In most situations, especially ordinary multiple regression, imputing "best guess" expected values for missing values results in biases. Deriving imputation models ignoring the response variable will bias final regression coefficients downward in absolute value. So it is usually better to develop imputations using the response variable to predict the independent variables, and to impute using randow values (random draws) for the predictors, i.e., to add random residuals into imputed values. You can easily obtain random draws using impute(x, 'random'), but these do not allow for relationships among predictors or between x and the response.

The aregImpute function generates multiple imputations without making distributional assumptions. After running aregImpute you can run the Hmisc fit.mult.impute function to fit the chosen model separately for each artifically completed dataset corresponding to each imputation. After fit.mult.impute fits all of the models, it averages the sets of regression coefficients and computes variance and covariance estimates that are adjusted for imputation using a standard formula. Here is an example:

Here fit.mult.impute fitted the 10 models using the built-in lm multiple regression function. A drawback to using lm here is that when you do summary(f) to get coefficients, standard errors, P-values, etc., only the coefficients are correct. Using the Design ols function in place of lm gets around this problem, and also allows for flexible ways to relax linearity assumptions. Here is an example:

4.8 Using S for Simulations and Bootstrapping

The S language and the ease of referencing the result of statistical functions makes S an ideal language for doing traditional Monte Carlo simulation as well as bootstrapping. When the dataset

forming the basis of the simulation is large or when the number of iterations is very large, S will run slower than other systems. However the savings in programming time usually more than makes up for the slower execution time.

For a first example let us use Monte Carlo simulation to estimate the population variance of the sample median for a sample of size n = 50 from a log-normal distribution. In the following code note the importance of setting aside **reps** locations in which to store the medians. If instead you set **meds** to NULL and continually concatenated sample medians to **meds** (e.g., **meds** \leftarrow c(meds, median(x)), the memory usage of the program would be very inefficient.

This took 1.8 seconds on a Pentium 166. Another approach would be to generate all the data up front, and to apply a matrix operation to compute the needed statistics:

This also took 1.8 seconds.

Now consider how to compute a simple bootstrap estimate (see also Section 4.7). Suppose the data consists of the heights in feet of a sample of 20 adults and we want to derive a 90% confidence interval for the population median height without making distributional assumptions. We take 500 samples with replacement, each of size 20, from the 20 heights, and compute the sample median. We then get the sample 0.05 and 0.95 quantiles of these 500 medians to form the desired confidence interval. The built–in sample function makes bootstrapping easy.

```
+ }
> table(meds)
5.1 5.25 5.3 5.4 5.45 5.5 5.55 5.6 5.65 5.7 5.7 5.75 5.8 5.8 5.85
  1 1 2 3 1 25 18 31
                                 40 8 88
                                             71 99
                                                     3
                                                         36
5.9 5.95 5.95 6 6.05 6.1 6.15
      5
         17 12
                 74
 27
                          1
> quantile(meds, c(.05, .95))
 5% 95%
5.5 5.95
```

This program ran in 3.9 seconds. The program can be shortened considerably because of built–in bootstrap functions:

> b ← bootstrap(h, median, B=B)
> limits.emp(b)

This ran in 5.0 seconds.

The **bootstrap** function is quite flexible. In the following example we use it to provide confidence limits for a type of estimate for which computing limits would be quite difficult by other means. We compute 0.95 confidence on the ranks of departments in a hospital, where what is being ranked is the mean satisfaction level with the departments, based on responses to a 5-point satisfaction scale. This is a common problem in "scorecarding" or "provider profiling" of departments, hospitals, or other entities. Just ranking the mean satisfaction scores across departments does not take into account the fact that the mean scores are estimates themselves. By using the bootstrap to derive confidence limits for ranks, we will lessen the chance that ranks will be misinterpreted. In what follows we stratify the overall analysis by the sex of the questionnaire's respondant.

First we do a more traditional analysis where individual mean satisfaction scores and t-based confidence limits are computed by department and by sex. The Hmisc summarize, smean.cl.normal, and Dotplot functions are useful. See Section 11.4.2 for more about Dotplot, which nicely displays results for dozens of departments along with "error bars", and see Section 11.4.3 for more examples of using summarize with trellis graphics functions. Here we downplay point estimates by using small tick marks (plus sign, pch=3) to mark them, and emphasize 0.99 confidence limits drawn with horizontal lines. The S reorder.factor function nicely orders the departments by the mean of the male and female satisfaction scores within each department. This makes the graph easier to read.

Next we analyze the data separately by sex to compute the ranks of the mean scores and 0.95 confidence limits for these ranks. We could use the **bootstrap** function easily by creating a data frame to contain department codes and satisfaction ratings, but it is faster to have **bootstrap** operate on a matrix. As the matrix (here, **d**) needs to be all numeric, we temporarily convert the

Department factor variable into integer codes. Factor levels are later re-associated with these codes for nice plotting. We use the group argument to bootstrap so that resampling is done separately within each department, to ensure that when these individual resamples are combined into one overall resample, each department's sample size equals the original sample size. After the bootstraps are done, results for both bootstraps are combined into a single data frame D.

```
> detach(1)
               # detach w, go back to raw data
# Define a function to compute stratified means and then rank them
# We can use this function for both overall ranks and ranks within
# bootstrap resamples. After all bootstrap resamples are done, we can
# use limits.emp to compute sample quantiles of these ranks,
# stratified by department
> rankdept \leftarrow function(d) {
   w \leftarrow tapply(d[,2], d[,1], mean, na.rm=T)
   r \leftarrow rank(w)
   names(r) \leftarrow names(w)
+
+
   r
+ }
> D \leftarrow NULL
> for(sx in levels(Sex)) {
   s \leftarrow Sex = sx
                    # analyze each sex separately
   d ← cbind(as.integer(Department)[s], Rating[s])
   ranks \leftarrow rankdept(d)
+
   +
   lim \leftarrow limits.emp(ranksb)
+
    w <-- data.frame(Sex=rep(sx,length(ranks)),
+
+
                    Department=
+
                     levels(Department)[as.integer(names(ranks))],
+
                    Rank=ranks,
+
                    Lower=lim[,1],
                                      # 0.025 quantile of 500 estimates
+
                    Upper=lim[,4]) # 0.975 quantile
+
    D \leftarrow rbind(D, w)
+ }
> # The 'as.integer(names(ranks))' trick uses the fact that we told
> # the rankdept function to retain the department codes as the names
> # attribute of the rank vector. Names are always stored as
> # character strings so we had to convert them to numeric
> # Arrange levels so that Dotplot will order categories by
> # average over female, male
> D$Department \leftarrow reorder.factor(D$Department, D$Rank, mean)
> Dotplot(Department \sim Cbind(Rank, Lower, Upper) | Sex,
+
          data=D, pch=3, xlab='Rank',
+
```

main='Ranks and 0.95 Confidence Limits for Mean Overall Satisfaction')

The analyst will usually find confidence limits for ranks to be quite wide, as they should be. Trying to rank small differences can be quite difficult.

4.8. USING S FOR SIMULATIONS AND BOOTSTRAPPING

Another place where bootstrapping ranks is useful is the situation where an investigator wishes to conclude that one predictor variable is better than another in terms of the Wald partial χ^2 minus the degrees of freedom (to level the playing field) contributed by the variables. The online help for the Design library's anova function has the following example, which uses the plot method for an anova.Design object without actually plotting the χ^2 s at each re-sample. We rank the negative of the adjusted χ^2 s so that a rank of 1 is assigned to the highest. It is important to tell plot.anova.Design not to sort the results, or every bootstrap replication would have ranks of 1,2,3 for the statistics.

```
> b ← bootstrap(mydata,
               rank(-plot(anova(
+
+
                lrm(y \sim rcs(x1,4)+pol(x2,2)+sex,mydata)), sort='none', pl=F)),
                B=50) # should really do B=500 but will take a while
+
> Rank \leftarrow b$observed
> lim \leftarrow limits.emp(b)[,c(1,4)] # get 0.025 and 0.975 quantiles
# Use the Hmisc Dotplot function to display ranks and their confidence
# intervals. Sort the categories by descending adj. chi-square, for ranks
sort='none', pl=F)
+
> predictor \leftarrow as.factor(names(original.chisq))
> predictor \leftarrow reorder.factor(predictor, -original.chisq)
> Dotplot(predictor \sim Cbind(Rank, lim), pch=3, xlab='Rank',
```

```
+ main='Ranks and 0.95 Confidence Limits for Chi-square - d.f.')
```

See the Hmisc bootkm function as another example of bootstrapping. For obtaining basic nonparametric confidence intervals for a population mean using the bootstrap percentile method as was used above, use the blazing fast smean.cl.boot function.

It is easy to call Fortran or C programs from within S. So if you are doing extensive simulations that run too slowly, you may want to isolate the slow code (particularly when subscripting must be done in a loop) and program it in Fortran or C.

For power simulations it is often very easy to program repeated regression model fitting. It is very important that you call the lowest possible level of fitting routine so that at each iteration S does not need to interpret model formulas, check for missing data, form design matrices, etc. Here is an example where we estimate the power for testing the effects of one predictor on a binary outcome, adjusted for another predictor. The population correlation between the two predictors is 0.75. The population regression coefficients are -1.4, 1, and 0.7, for the intercept and two predictors, respectively. This program simulates power unconditional on x1 and x2. To simulate conditional power, generate these variables once before the loop.

store()

```
← 50
n
nsim \leftarrow 1000
rho \leftarrow .75
\texttt{beta1} \ \leftarrow \ \texttt{1}
beta2 \leftarrow .7
intercept \leftarrow -1.4
# Show inter-quartile-range odds ratios in effect
cat('IQR OR for adjustor:',format(exp(beta1*1.34898)),'\n')
cat('IQR OR for predictor:',format(exp(beta2*1.34898)),'\n')
r \leftarrow prop \leftarrow chisq \leftarrow single(nsim)
for(i in 1:nsim) {
  cat(i,'')
  x1 \leftarrow rnorm(n) # unconditional power on x1,x2
  x2 \leftarrow rnorm(n) + (rho/sqrt(1 - rho*rho)) * x1
  L \leftarrow intercept+beta1*x1+beta2*x2
  y \leftarrow ifelse(runif(n) \leq plogis(L), 1, 0) \# or better:
  y \leftarrow rbinom(n, size = 1, prob = plogis(L))
  r[i] \leftarrow cor(x1,x2)
  prop[i] \leftarrow mean(y)
  x \leftarrow cbind(x1, x2)
  f \leftarrow lrm.fit(x,y) # lrm.fit in Design, called by lrm
  chisq[i] \leftarrow (f$coef[3])^2/f$var[3,3]
J
prn(mean(r),'Mean correlation between x1 and x2') # prn in Hmisc
prn(mean(prop),'Mean proportion Y=1')
prn(mean(chisq>3.84),'Power')
```

For some problems you may have sample predictor values in a previous study. If the sample size used in the simulation is less than that from the previous study, you can form the x1,x2 vectors

by sampling without replacement from the study's values. Otherwise, you might consider sampling with replacement. Either of these approaches will allow you to use actual rather than hypothetical normal distributions. There is still the problem of what population regression coefficient values to use in the simulations. Here is an example.

See Section 5.3 for an example where the Hmisc **spower** function is used to simulate the power of a survival time comparison. See Section 7.2.1 for an example where multivariate normal repeated measurement data are simulated.

Chapter 5

Probability and Statistical Functions

5.1 Basic Functions for Statistical Summaries

There are many functions to produce statistical summaries. We already used describe and table. Table 5.1 gives a concise list of some other basic functions. All the functions below pmax are in the Hmisc library.

A few details about these functions: cor computes the ordinary Pearson product-moment linear correlation coefficient. cor,mean,var,median, min, max, and quantile do not accept NAs without extra effort. The cor.test function will automatically exclude NAs. All but var and cor have an optional parameter na.rm which can be set to T to cause NAs to be deleted before doing any calculations. For var and cor you will have to delete the NAs from the input variables yourself. mean and median do not operate separately in columns of matrices. Use a combination of the function and apply for this purpose. min and max have the same limitation as mean, but pmin and pmax can be used to obtain the min or max of several vectors simultaneously.

rcorr efficiently computes Pearson and Spearman rank correlation matrices and P-values, doing pairwise deletion of NAs. hoeffd uses pairwise deletion of NAs in computing Hoeffding's general measure of dependence between any two variables.

The functions bystats and bystats2 in Hmisc can be used to obtain statistics on a variable by the levels of several classification variables (i.e., by-processing). These have been superceded to some extent by Hmisc's summary.formula and summarize functions, but bystats can still be useful for stratification by more than two variables. See Section 6.2 for examples of summary.formula.

Comments Function Description cor cor(x,y) correlations between \mathbf{x} and \mathbf{y} cor.test cor.test(x,y,method) Pearson, Spearman, Kendall corr. and tests variances and covariances var(x,y) var cumsum(x) cumulative sums cumsum mean mean(x)mean of a vector median median median of a vector quantile quantile(x,probs=...) quantiles overall minimum value of all arguments min min(...) max(...) overall maximum value of all arguments max pmin pmin(...) minimum for each row over several vectors pmax pmax(...) maximum for each row over several vectors describe describe(..) describe data frame or any type of var. bystats(y,...,fun=...) stratified statistics bystats flexible stratified statistics summary.formula summary(y \sim ...) summarize(x,byvar,FUN) multi-way stratified statistics summarize make dummies to summarize ordinal y cumcategory cumcategory(y) binconf(successes,events,alpha) exact and Wilson C.L. for probability binconf smean.cl.normal smean.cl.normal(y) compute normal (t) C.L. smean.sd(y)mean and std. dev. smean.sd smean.sdl smean.sdl(y) mean \pm constant \times s.d. smean.cl.boot smean.cl.boot(y) nonparametric boot. C.L. for mean smedian.hilow(y) smedian.hilow median and 2 symmetric tailed quantiles hoeffd hoeffd(x,y) Hoeffding D statistic rcorr rcorr(...) linear or rank correlation matrix Somers D_{xy} rank correlation rcorr.cens rcorr.cens(...) for censored data rcorrp.cens(...) modification of rcorrp.cens rcorrp.cens for paired predictors bootkm(S,q=,times=) Bootstrap Kaplan-Meier bootkm estimates

Table 5.1: Functions for Statistical Summaries

5.1. BASIC FUNCTIONS FOR STATISTICAL SUMMARIES

> bystats(age,stage,status,fun=quantile)

quantile of age by stage, status

| | Ν | Missing | 0% | 25% | 50% | 75% | 100% |
|--------------------------------|-----|---------|----|-------|------|-------|------|
| 3 alive | 96 | 0 | 49 | 67.75 | 72.0 | 74.00 | 83 |
| 4 alive | 51 | 1 | 50 | 68.00 | 72.0 | 75.00 | 84 |
| 3 dead - prostatic ca | 35 | 0 | 55 | 66.50 | 72.0 | 74.50 | 78 |
| 4 dead - prostatic ca | 95 | 0 | 49 | 64.00 | 73.0 | 76.00 | 82 |
| 3 dead - heart or vascular | 66 | 0 | 54 | 71.00 | 73.0 | 76.00 | 88 |
| 4 dead - heart or vascular | 30 | 0 | 68 | 71.00 | 73.0 | 75.00 | 87 |
| 3 dead - cerebrovascular | 21 | 0 | 62 | 72.00 | 75.0 | 76.00 | 80 |
| 4 dead - cerebrovascular | 10 | 0 | 48 | 72.25 | 74.0 | 76.00 | 78 |
| 3 dead - pulmonary embolus | 10 | 0 | 68 | 70.50 | 76.0 | 79.00 | 83 |
| 4 dead - pulmonary embolus | 4 | 0 | 62 | 68.75 | 74.0 | 77.25 | 78 |
| 3 dead - other ca | 20 | 0 | 51 | 72.00 | 74.5 | 76.00 | 80 |
| 4 dead - other ca | 5 | 0 | 66 | 72.00 | 73.0 | 73.00 | 76 |
| 3 dead - respiratory disease | 12 | 0 | 59 | 72.00 | 75.0 | 81.00 | 89 |
| 4 dead – respiratory disease | 4 | 0 | 70 | 73.75 | 76.0 | 77.75 | 80 |
| 3 dead - other specific non-ca | 19 | 0 | 62 | 68.50 | 76.0 | 78.00 | 81 |
| 4 dead - other specific non-ca | 9 | 0 | 61 | 71.00 | 72.0 | 73.00 | 83 |
| 3 dead - unspecified non-ca | 3 | 0 | 73 | 73.50 | 74.0 | 76.00 | 78 |
| 4 dead - unspecified non-ca | 4 | 0 | 71 | 71.75 | 75.5 | 79.25 | 80 |
| 3 dead - unknown cause | 7 | 0 | 52 | 64.50 | 71.0 | 73.00 | 76 |
| ALL | 501 | 1 | 48 | 70.00 | 73.0 | 76.00 | 89 |

The default value for fun is mean.

Several statistical summary functions are useful with summary.formula, summarize, tapply, apply, and by themselves. These functions (cumcategory through smedian.hilow in the table) provide statistical summaries for printing and plotting (including "error bars"; see Section 11.4.3). Here are some examples based on a sample of size 500 from a uniform(0,1) distribution:

```
> set.seed(2) # so can replicate example
> x \leftarrow runif(500)
> smean.cl.normal(x)
 Mean Lower Upper
0.501 0.475 0.527
> smean.cl.boot(x)
 Mean Lower Upper
0.501 0.476 0.526
> smean.sd(x)
 Mean SD
0.501 0.292
> smean.sdl(x)
> # mean +- 2 s.d. (smean.sdl(x,1) to get mean +- s.d.)
 Mean Lower Upper
0.501 -0.0831 1.08
> smedian.hilow(x)
> # median and .025, .975 quantiles (conf.int=.5 for quartiles)
Median Lower Upper
```

0.522 0.0201 0.971

The rcorr.cens, rcorrp.cens, and bootkm functions in Hmisc are used with right-censored failure-time data. The first two compute rank correlation measures for censored response data, and bootkm bootstraps Kaplan-Meier survival probability or quantile estimates. The help files for these functions give more information.

5.2 Functions for Probability Distributions

For each distribution in Table 5.2, four functions are available: one for densities, one for cumulative distribution functions, one for quantiles and one to obtain random samples from that distribution. Add the prefixes d, p, q or r to the Name column to get the name of the desired function. Functions in Hmisc related to probability distributions include ecdf (which plots the step-function empirical cumulative distribution function of a vector or of all the continuous variables in a data frame) and bpplot (box-percentile plots). See Section 11.3 for more about these as well as information about the Hmisc scat1d and histSpike functions for drawing rug plots, histograms, and density estimates.

| Name | Parameters |
|---------|--|
| beta | shape1 |
| | shape2 |
| binom | size |
| | prob |
| cauchy | location |
| | scale |
| chisq | df |
| exp | rate |
| f | df1 |
| | df2 |
| gamma | shape |
| geom | shape |
| lnorm | meanlog |
| | sdlog |
| logis | location |
| | scale |
| nbinom | size |
| | prob |
| norm | mean |
| | sd |
| - | lambda |
| t | df |
| unif | min |
| | max |
| weibull | shape |
| | |
| bpplot | list of vectors |
| | beta binom cauchy chisq exp f gamma geom lnorm logis nbinom norm pois t unif |

 Table 5.2: Probability Distribution Functions

Here are some examples.

```
# Compute the probability of getting 3 or fewer heads out of 10
# tosses of a fair coin
> pbinom(3, 10, .5)
[1] 0.171875
# Use the Hmisc function binconf to compute an exact 0.99 confidence
# interval for the unknown probability of an event given 6 events
# were observed out of 10 trials. The Wilson score test-based
# interval has been shown to offer more accurate coverage than the
# exact beta-distribution-based method. It's often the case that
# so-called 'exact' methods are conservative (Fisher's exact test for
# comparing two proportions can be quite conservative)
> binconf(6, 10, .01)
       Lower Upper
Exact 0.191 0.923
Wilson 0.248 0.872
# Do an F-test to test HO: two variances are equal, given
# a sample standard deviation of 35.6 from n=100 and an
# s.d. of 17.3 from n=74. See Rosner 4th Edition Ex. 8.15 P. 268
> vratio ← (35.6/17.3)<sup>2</sup>
> vratio
[1] 4.234555
> 2*(1 - pf(vratio, 99, 73)) # 2-tailed P-value
[1] 8.612535e-010
# Compute a 0.95 confidence interval for the population variance ratio
> ratios \leftarrow qf(c(.025,.975), 99, 73)
> ratios
[1] 0.654760 1.549079
> vratio/ratios
[1] 6.467339 2.733596
```

Had we been using the raw data for the last example, the calculations could have been done using the S builtin function var.test if we provided it the raw data. We can thankfully work backwards to generate raw data having the needed mean and standard deviation, just so we can use var.test. The following function will generate a vector of length n having sample mean and standard deviation exactly equal to given constants. After the appropriate vectors are computed we can use var.test.

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```
> mean(y1)
[1] 3.552714e-016
> sqrt(var(y1))
[1] 35.6
> y2 \leftarrow gen.mean.sd(74, sd=17.3)
> var.test(y1,y2)
    F test for variance equality
data: y1 and y2
F = 4.2346, num df = 99, denom df = 73, p-value = 0
alternative hypothesis: true ratio of variances is not equal to 1
95 percent confidence interval:
2.733596 6.467339
sample estimates:
variance of x variance of y
       1267.36
                      299.29
```

5.3 Hmisc Functions for Power and Sample Size Calculations

Table 5.3 lists functions in Hmisc related to statistical power.

| | · / 1 |
|-------------|---|
| Function | Purpose |
| ballocation | Find optimum allocation ratio for |
| | treatments for binary responses |
| bpower | Power of two–sample binomial test |
| | (approximate; for comparing two proportions) |
| bpower.sim | Power of two-sample binomial test |
| | using simulation |
| bsamsize | Sample size for two–sample binomial test |
| ciapower | Power of interaction test for exponential |
| | survival (and for Cox model) |
| cpower | Power of Cox/log-rank two-sample Test |
| gbayes | Gaussian Bayesian posterior and predictive |
| | distributions (and simple conditional power dist.) |
| popower | Power for two–sample test for ordinal responses |
| posamsize | Sample size for two–sample ordinal responses |
| | Sample size for 2-sample binomial using |
| | $\sin^{-1}\sqrt{p}$ transformation (by Rick Chappell) |
| spower | Power of Cox/log-rank two-sample test for |
| | complex situations via simulation |

Table 5.3: Hmisc Functions for Power/Sample Size

The ballocation, bpower.sim and bsamsize functions are documented under the heading of the bpower function. posamsize is listed under popower.

In the following example, both the **bpower** and **bpower.sim** functions are used to estimate power for the two-sample binomial test (comparison of two proportions). **bpower.sim** can simulate power of the χ_1^2 test very quickly because S has a builtin binomial random number generator. By default, 10000 simulations are done (this takes about 5 seconds). 0.95 confidence limits for the estimated power based on the simulations are reported.

```
> args(bpower)
function(p1, p2, odds.ratio, percent.reduction, n, n1, n2, alpha = 0.05)
> args(bpower.sim)
function(p1, p2, odds.ratio, percent.reduction, n, n1, n2, alpha = 0.05,
        nsim = 10000)
> bpower(.2, odds.ratio=2, n=200)
    Power
0.5690973
> bpower.sim(.2, odds.ratio=2, n=200)
 Power
           Lower
                    Upper
 0.5581 0.5483664 0.5678336
> bpower.sim(.2, odds.ratio=2, n=200, nsim=25000)
   Power
           Lower
                       Upper
0.56256 0.5564106 0.5687094
> args(bsamsize)
function(p1, p2, fraction = 0.5, alpha = 0.05, power = 0.8)
> bsamsize(.2, plogis(qlogis(.2)+log(2)), power=.5690973)
      n1
                n2
100.0041 100.0041
```

Note that **bsamsize** does not allow specification of an odds ratio. We used the logistic and inverse logistic transform to get the second proportion by applying an odds of 2 to the first proportion (.2).

Next we compute power for a proportional odds two-sample test for comparing two ordinal responses. The first calculation is for an ordinal response with only two levels. Power for this situation should be close to the 0.56 just computed, but in fact it is different, as **popower** uses a normal approximation for the log odds ratio instead of subtracting the two proportions. This approximation is not as good as the method used by **bpower** when there are two categories. For each application of **popower** we assume that the marginal frequencies of responses are equal across response categories. You can see that when more ordered categories are used, the power increases (especially when the cell frequencies are equal).

```
> args(popower)
function(p, odds.ratio, n, n1, n2, alpha = 0.05)
> popower(c(.5,.5), 2, 200)
Power: 0.684
Efficiency of design compared with continuous response: 0.75
> popower(c(1,1,1)/3, 2, 200)
Power: 0.756
Efficiency of design compared with continuous response: 0.889
> popower(c(1,1,1,1)/4, 2, 200)
Power: 0.778
```

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Efficiency of design compared with continuous response: 0.938

> popower(c(1,1,1,1,1)/5, 2, 200)
Power: 0.788
Efficiency of design compared with continuous response: 0.96

In the next example, taken from the **bpower** help file, we plot power vs. the total sample size n for various odds ratios, using 0.1 as the probability of the event in the control group. A separate curve is plotted for each odds ratio, and the odds ratio is drawn just below the curve at n = 350.

```
n ← seq(10, 1000, by=10)
OR ← seq(.2,.9,by=.1)
plot(0, 0, xlim=range(n), ylim=c(0,1), xlab="n", ylab="Power", type="n")
for(or in OR) {
    lines(n, bpower(.1, odds.ratio=or, n=n))
    text(350, bpower(.1, odds.ratio=or, n=350)-.02, format(or))
}
```

Now re-do the plot, letting Hmisc's **labcurve** function do the work of drawing the curves, determining overall axis limits, and labeling curves at points of maximum separation.

The cpower function for estimating power for the Cox/log-rank two-sample test has many options that allow a time-to-event study to have several complexities. Here is an excerpt from the help file.

DESCRIPTION

Assumes exponential distributions for both treatment groups. Uses the George-Desu method along with formulas of Schoenfeld that allow estimation of the expected number of events in the two groups. To allow for drop-ins (noncompliance to control therapy, crossover to intervention) and noncompliance of the intervention, the method of Lachin and Foulkes is used.

USAGE

REQUIRED ARGUMENTS

```
tref time at which mortalities estimated
n total sample size (both groups combined). If allocation is unequal
so that there are not n/2 observations in each group, you may
```

```
specify the sample sizes in nc and ni.

mc tref-year mortality, control

r % reduction in mc by intervention

accrual duration of accrual period

tmin minimum follow-up time
```

```
OPTIONAL ARGUMENTS
```

| noncomp.c | % non-compliant in control group (drop-ins) |
|-----------|---|
| noncomp.i | % non-compliant in intervention group (non-adherers) |
| alpha | type I error probability. A 2-tailed test is assumed. |
| nc | number of subjects in control group |
| ni | number of subjects in intervention group. |
| | nc and ni are specified exclusive of n. |
| pr | set to F to suppress printing of details |

The help file for **cpower** has an example in which 4 plots are drawn on one page, one plot for each combination of noncompliance percentage. Within a plot, the 5-year mortality % in the control group is on the x-axis, and separate curves are drawn for several % reductions in mortality with the intervention. The accrual period is 1.5y, with all patients followed at least 5y and some 6.5y.

The spower function is much slower than cpower as it relies on simulation, but it allows for very complex clinical trial setups. cpower works with Quantiles2 and other functions documented under the spower heading. The following paragraph is taken from spower's help file:

Given functions to generate random variables for survival times and censoring times, spower simulates the power of a user-given 2-sample test for censored data. By default, the logrank (Cox 2-sample) test is used, and a logrank function for comparing 2 groups is provided. For composing S functions to generate random survival times under complex conditions, the Quantile2 function allows the user to specify the intervention:control hazard ratio as a function of time, the probability of a control subject actually receiving the intervention (dropin) as a function of time, and the probability that an intervention subject receives only the control agent as a function of time (non-compliance, dropout). Quantile2 returns a function that generates either control or intervention uncensored survival times subject to non-constant treatment effect, dropin, and dropout. There is a plot method for plotting the results of Quantile2, which will aid in understanding the effects of the two types of non-compliance and non-constant treatment effects. Quantile2 assumes that the hazard function for either treatment group is a mixture of the control and intervention hazard functions, with mixing proportions defined by the dropin and dropout probabilities. It computes hazards and survival distributions by numerical differentiation and integration using a grid of (by default) 7500 equally-spaced time points.

Besides providing the Quantile2 function, the spower package also contains three functions which compose S functions that compute survival probabilities for Weibull, log-normal, and Gompertz distributions. These functions (Weibull2,Lognorm2, and Gompertz2) work by solving for the two parameters of each of these distributions which make them fit two user-specified times and survival probabilities. The 3 types of functions so created are useful as the first argument to Quantile2.

The following example demonstrates the flexibility of **spower** and related functions. We simulate a 2-arm (350 subjects/arm) 5-year follow-up study for which the control group's survival distribution is Weibull with 1-year survival of .95 and 3-year survival of .7. All subjects are followed at

```
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```

least one year, and patients enter the study with linearly increasing probability starting with zero. Assume (1) there is no chance of dropin for the first 6 months, then the probability increases linearly up to .15 at 5 years; (2) there is a linearly increasing chance of dropout up to .3 at 5 years; and (3) the treatment has no effect for the first 9 months, then it has a constant effect (hazard ratio of .75).

```
> # First find the right Weibull distribution for compliant control patients
> # Weibull2 is bundled with spower
> sc \leftarrow Weibull2(c(1,3), c(.95,.7))
> sc
function(times, alpha = 0.0512932943875506, gamma = 1.76519490623438
  )
   exp( - alpha * (times^gamma))
> # Inverse cumulative distribution for case where all subjects are followed
> # at least a years and then between a and b years the density rises
> # as (time - a) \hat{d} is a + (b-a) * u \hat{d} (1/(d+1))
> rcens \leftarrow function(n) 1 + (5-1) * (runif(n) ^ .5)
> # To check this, type hist(rcens(10000), nclass=50)
> # Put it all together
> f <- Quantile2(sc,
                 hratio=function(x)ifelse(x <= .75, 1, .75),
+
+
                 dropin=function(x)ifelse(x <= .5, 0, .15*(x-.5)/(5-.5)),
                 dropout=function(x).3*x/5)
> par(mfrow=c(2,2)) # 2x2 matrix of plots
> plot(f, 'all', label.curves=list(keys='lines'))
> #omitting label.curves= will cause labcurve to label curves directly
```

The function f created by Quantile2 has as its main arguments n, the number of random variates to draw, and what, telling the function whether to draw samples from the uncensored survival times for control or intervention. The plot(f,...) statement produced Figure 5.1.

Now we ask **spower** to simulate the needed results, basing the survival distribution comparison on the log-rank test.

See Section 4.8 for an example in which power for a logistic model is estimated via simulation.

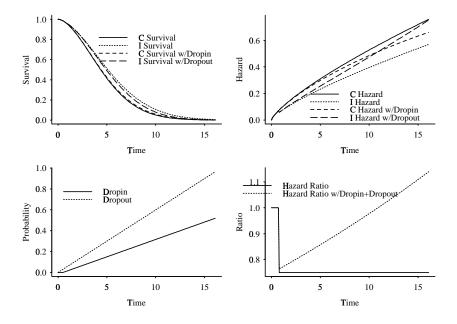


Figure 5.1: Characteristics of control and intervention groups with a lag in the treatment effect and with non-compliance in two directions

5.4 Statistical Tests

In general, we do not prefer to use specialized functions for many of the common statistical tests for three reasons. (1) Many tests are special cases of regression models. (2) The notation used in regression models unifies many of the concepts involved in statistical inference. (3) Regression models can provide estimates of effects, not just tests of (sometimes inappropriate) null hypotheses. Regarding point (2), the two-sample t-test is a special case of the linear regression model with a single binary predictor variable. The two-sample Wilcoxon test is a special case of the proportional odds ordinal logistic model again with a single binary predictor. The two-sample Wilcoxon test is also a special case of the Spearman rank correlation test. The k-sample generalizations of these tests (analysis of variance and Kruskal–Wallis test) may be obtained by using the two above mentioned regression models with k - 1 dummy variables. The χ^2 test for a $k \times 2$ contingency table is a special case of a binary logistic model with k - 1 dummy predictors, and the likelihood ratio χ^2 test from this model yields P-values that are more accurate than the traditional χ^2 test. The log-rank test is a special case of the Cox model.

The entire list of statistical tests builtin to S-PLUS may be obtained under Microsoft Windows by clicking under Index and entering Statistical Inference. You can also get the list by typing the command help('Statistical Inference'). Table 5.4 lists these functions.

| Description | Function |
|--|-----------------|
| χ^2 Goodness–of–fit | chisq.gof |
| Exact binomial 1–sample | binom.test |
| F test for variances | var.test |
| Fisher's exact test for $p \times q$ table | fisher.test |
| Friedman rank sum | friedman.test |
| Graph two cumulative distributions | cdf.compare |
| Kolmogorov–Smirnov goodness–of–fit | ks.gof |
| Kruskal–Wallis rank sum | kruskal.test |
| Mantel–Haenszel χ^2 | mantelhaen.test |
| McNemar χ^2 | mcnemar.test |
| Pearson χ^2 | chisq.test |
| Proportion tests | prop.test |
| Student t | t.test |
| Correlation | cor.test |
| Wilcoxon 1– and 2–sample | wilcox.test |

 Table 5.4: S Functions for Statistical Tests

It is not clear why Fisher's exact test is implemented in S, as this test is known to lose power when compared with unconditional χ^2 tests¹

¹Note that the "rule" that ordinary χ^2 tests should not be used when an expected cell frequency is < 5 is not correct. Pearson χ^2 works well in situations more extreme than that, and the likelihood ratio χ^2 may work even better.

5.4.1 Nonparametric Tests

The Spearman correlation test (and hence the two-sample Wilcoxon test) may be obtained using the Hmisc spearman.test function:

```
> set.seed(17) # so can reproduce results
> sex ~ factor(sample(c('female', 'male'),100,T))
> blood.pressure ~ rnorm(100, 100, 8)+3*(sex=='male')
> options(digits=3)
> spearman.test(sex, blood.pressure)
Rsquare F df1 df2 pvalue n
    0.0713 7.52 1 98 0.00725 100
```

You can also obtain the Spearman test from the Hmisc rcorr function [better still, S has a builtin function cor.test that does Spearman and Pearson linear correlation tests]. Note that $0.27^2 = 0.071$ and the two methods give identical two-tailed *P*-values.

The Hmisc **somers2** function provides a more easily interpreted correlation measure for the case where one variable is binary. Here Somers' D_{xy} rank correlation between x=blood pressure and y=sex is computed, along with the probability of concordance between the two variables denoted by C.

```
> somers2(blood.pressure,sex='male')
        C Dxy n Missing
    0.654 0.308 100 0
```

The Hmisc rcorr.cens can also compute this correlation as a special case where censoring is absent.

```
> rcorr.cens(blood.pressure,sex)
C Index Dxy S.D. n missing uncensored Relevant Pairs Concordant Uncertain
    0.654 0.308 0.109 100 0 100 4992 3266 0
```

This can be used to get a statistical test using a normal approximation. Here we compute the two-tailed P-value.

```
> (1-pnorm(.308/.109))*2
[1] 0.00471
>
```

spearman.test can also test for non-monotonic relationships between two continuous variables, by allowing the user to specify an order of the polynomial of the ranks used in the correlation test. For example, to get a two d.f. test of association between age and blood pressure, allowing for one "turn" in the non-monotonic function, one could use **spearman.test(age, blood.pressure, 2)**.

The spearman2 function in Hmisc is the most general of the Spearman-type functions. It uses the F approximation to do a Spearman and second-order generalized Spearman test (as done by spearman.test, if the predictor variable is continuous), the Wilcoxon-Mann-Whitney two-sample test, and the Kruskal-Wallis test (for factor predictors having more than 2 levels). spearman2 can test a series of predictors against a common response variable, with pairwise deletion of missing data. Here is an example in which the numerator degrees of freedom are 1, 1, and 4, respectively, for age (continuous), sex (binary), and race (5 levels).

```
> spearman2(blood.pressure ~ age + sex + race)
```

The S builtin function wilcox.test has more features for one²- and two-sample Wilcoxon tests. It's use is somewhat awkward for the two-sample case:

> wilcox.test(blood.pressure[sex=='female'], blood.pressure[sex=='male'])

```
data: blood.pressure[sex == "female"] and blood.pressure[sex == "male"]
rank-sum normal statistic with correction Z = -2.65, p-value = 0.008
alternative hypothesis: true mu is not equal to 0
```

For a one-sample test, omit the second argument to wilcox.test.

Next obtain the two–sample Wilcoxon test as a special case of the proportional odds model. This approach will give very accurate P-values (as well as an effect measure — the odds ratio) although it takes computer time and RAM to fit 99 intercepts for the 100 observations that contain no tied response values³

```
> library(Design, T)
> lrm(blood.pressure \sim sex)
Obs Max Deriv Model L.R. d.f.
                                  Ρ
                                        С
                                            Dxy Gamma Tau-a
                                                              R2 Brier
100
       5e-013
                    7.27
                            1 0.007 0.578 0.156 0.308 0.156 0.07 0.01
                               S.E. Wald Z
                                                Ρ
                        Coef
y>=83.1881961293538 4.214947 1.0140 4.16 0.0000
y>=85.4474231763989 3.511529 0.7269 4.83 0.0000
y>=86.1909623865412 3.092591 0.6018 5.14 0.0000
. . . . .
y>=116.829586001076 -4.065680 0.6321 -6.43 0.0000
y>=118.266935916644 -4.485844 0.7529 -5.96 0.0000
y>=119.44799460213 -5.193478 1.0332 -5.03 0.0000
          sex=male 0.951687 0.3569 2.67 0.0077
```

The Wald test P-value is 0.008 and the somewhat more accurate likelihood ratio test yields P=0.007, in good agreement with what we obtained from the simpler tests. The D_{xy} rank correlation printed above does not agree with the earlier ones because we have reversed the roles of x and y.

²Wilcoxon signed–rank test

 $^{^{3}}$ Note that there are no statistical problems in fitting 100 parameters for 100 observations here, as the intercepts are constrained to be in order.

Various other nonparametric testing functions are listed in table 5.4. These include tests for goodness–of–fit, frequencies, proportions, blocked data, and tests for distributional shapes.

5.4.2 Parametric Tests

The t test may be obtained using the builtin t.test function.

```
> t.test(blood.pressure[sex=='female'], blood.pressure[sex=='male'])
```

```
Standard Two-Sample t-Test
```

```
data: blood.pressure[sex == "female"] and blood.pressure[sex == "male"]
t = -2.6769, df = 98, p-value = 0.0087
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
    -6.82129 -1.01326
sample estimates:
    mean of x mean of y
    98.656 102.573
```

Consider Example 8.20 on P. 275 of Rosner (4th Edition) in which the hospital dataset is used. Here we test for zero mean difference (why the mean?) in duration of hospitalization, for patients receiving an antibiotic compared with those who didn't.

```
> attach(hospital)
> t.test(duration[antibiotic=='yes'],duration[antibiotic=='no'])
    Standard Two-Sample t-Test
data: duration[antibiotic == "yes"] and duration[antibiotic == "no"]
t = 1.6816, df = 23, p-value = 0.1062
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
    -0.9497745 9.2037428
sample estimates:
    mean of x mean of y
    11.57143 7.444444
```

Note that the confidence interval does not agree with Rosner's calculations, as Rosner inappropriately used 6 d.f. for the t distribution instead of 23 d.f. In S-PLUS 4.x these results may be obtained using the menus: Statistics .. Compare Samples .. Two Samples .. t-test; use antibiotic as a grouping variable.

Now consider a one-sample t-test using the data on the effects of oral contraceptive (OC) on systolic blood pressure found in Rosner Table 8.1 on P. 253. Here is a listing of the data file named table81.asc:

sbp.noOC sbp.OC 115 128 112 115 107 106

| 119 | 128 |
|-----|-----|
| 115 | 122 |
| 138 | 145 |
| 126 | 132 |
| 105 | 109 |
| 104 | 102 |
| 115 | 117 |

Note that variable names are in the first record. Here fields are separated by a tab. In S-PLUS 4.x we may import this data file using File ... Import Data ... From File ... and then browsing to find the file. Then click OK, using all defaults. Under any version of S we may import the data using the command

The one–sample *t*–test and associated confidence interval for the difference in means may be obtained as follows:

```
> t.test(sbp.OC,sbp.noOC,paired=T)
```

Paired t-Test

```
data: sbp.OC and sbp.noOC
t = 3.3247, df = 9, p-value = 0.0089
alternative hypothesis: true mean of differences is not equal to 0
95 percent confidence interval:
1.533987 8.066013
sample estimates:
mean of x - y
4.8
```

Under S-PLUS 4.x you can use Statistics ... Compare Samples ... Two Samples ... t Test. Check the box marked Paired t. Had you already computed a new variable containing the difference in the two columns, you could use Statistics ... Compare Samples ... One Sample ... t Test.

Other parametric testing functions are shown in Table 5.4. These include tests for equality of variances and tests for zero correlations (why zero?).

Chapter 6

Making Tables

6.1 S-PLUS-supplied Functions

Section 4.3.2 showed how to use functions such as tapply to make simple tables. The S print.char.matrix function may be used to format many tables into attractively boxed cells. The crosstabs function produces frequency tables and computes Pearson χ^2 statistics, printing results using print.char.matrix. Here is an example from the online help, using the S-PLUS-supplied solder dataset.

> crosstabs(\sim Solder+Opening, data=solder, subset = skips>10) Call:

```
crosstabs( \sim Solder + Opening, data = solder, subset = skips > 10)
158 cases in table
+----+
N
         1
|N/RowTotal|
N/ColTotal
|N/Total |
+----+
Solder |Opening
      S
           ΙM
                   L
                           |RowTotl|
     _+____
                   -+----
                         --+----+
Thin
    199
            115
                   19
                           1123
                                  Т
      0.805 0.122 0.073 0.78
                                  T
      |0.805 |0.577
                   1.000
                          0.627 0.095 0.057
                          T
----+---+----+----+----+----+---
                                 -+
Thick |24
             |11
                   0
                           135
                                  Т
      0.686 0.314 0.000 0.22
                                  1
      0.195 0.423 0.000
                                  1
      0.152 0.070 0.000
                                  1
_____+
                          _+___
                               ---+
ColTotl|123
            26
                   19
                           158
                                  1
     0.778 0.165 0.057
                          - I
                                  Т
----+
Test for independence of all factors
   Chi<sup>2</sup> = 9.18309 d.f.= 2 (p=0.01013719)
   Yates' correction not used
   Some expected values are less than 5, don't trust stated p-value
```

Note that the first argument to **crosstabs** is an S *formula*. Normally a formula has a dependent or response variable followed by a tilde followed by one or more independent or predictor variables, separated by "+". A contingency table as such does not have a response variable as it treats row and column variables symmetrically. Therefore a formula given to **crosstabs** specifies only a series of "independent" variables. Functions which operate on formulas provide a number of advantages:

- 1. Formulas allow the user to specify any number of variables to analyze.
- 2. Functions which use formulas also allow for an argument called data that specifies a data frame or list that contains the analysis variables. You need not attach the data frame to get access to these variables.
- 3. Functions which use formulas also allow the user to specify a **subset** argument, to easily specify that an analysis is to be run on a subset of the observations. The value specified to **subset** is a logical vector or a vector of integer subscripts.

The object created by **crosstabs** contains much useful information including marginal summaries that can be plotted. Let's re–run the last table, saving the result and then printing part of it.

```
> g \leftarrow crosstabs( \sim Solder + Opening, data = solder, subset = skips > 10)
```

```
> rowpct ~ 100*attr(g,'marginals')$"N/RowTotal"
```

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The rowpct matrix contains the row percentages, as can be seen by comparing with the full table above. To plot these row percents using trellis graphics (see Section 11.4) we first need to reshape the rowpct matrix into a a vector as was done in Section 4.3.9:

```
\leftarrow as.vector(rowpct)
                                 # strung-out vector
> y
> Solder ~ dimnames(rowpct)[[1]][row(rowpct)]
> Opening ← dimnames(rowpct)[[2]][col(rowpct)]
> data.frame(Solder, Opening, y)
  Solder Opening
                    y
   Thin
         S 80.49
1
              S 68.57
2 Thick
3
   Thin
             M 12.20
4 Thick
              M 31.43
              L 7.32
  Thin
5
6 Thick
              L 0.00
> dotplot(Solder \sim y | Opening)
> dotplot(Solder \sim y, groups=Opening, panel=panel.superpose)
> barchart(Opening \sim y | Solder)
```

The second dot plot is probably more effective, as the sum of values indicated by all the points on each line is 100%. The Hmisc **reShape** function provides a shortcut:

Note that you can also compute row or column proportions or percents using the table, apply, and sweep functions.

6.2 The Hmisc summary.formula Function

The summary.formula function (called using the summary command on a formula object) constructs a large variety of tables of descriptive statistics. The tables can automatically be typeset using LAT_EX. The default format for typesetting tables this way is the "Biometrika/New England Journal of Medicine" format, i.e., it makes minimal use of vertical lines.

Some of the tables can automatically be converted into dot charts by one of summary.formula's plot methods.

Part of what makes summary.formula work is that the user can specify her own function (fun) to compute descriptive statistics¹ and this function may be multivariate. For example, it may operate on two response variables, producing two or more summary statistics, or it may compute a single summary statistic on the two responses. If the two responses are a survival time and an event/censoring indicator, you can summarize the survival times using Kaplan–Meier or other estimators. If the two responses are the predicted probability of a disease and whether or not the disease is actually present, the summary measure could be a "receiving operator characteristic curve area." You can also specify that fun is to return several statistics from each response variable (e.g., mean and median).

In addition to its flexibility, summary.formula has two general advantages over builtin S functions. First, it removes NAs before passing vectors to standard S statistical functions (mean, median, etc.) so that you do not need to worry about using an na.rm=T argument. Second, statistical summaries made by summary.formula automatically include *marginal* summaries. For example, if you stratify data on a variable you will also see unstratified estimates, and if you cross-classify on two or more variable you will also see estimates stratified on all subsets of the variables. Thus cross-classifying on race and sex and computing the median cholesterol will (unless you specify an argument to suppress them) also compute medians stratified separately by race and by sex as well as the grand median cholesterol.

There are three major ways of using summary.formula, as defined by the method parameter. method='response' (the default) causes the function to summarize one or more response variables separately by levels of any number of right-hand-side variables. method='cross' results in a multiway breakdown. Categorical right-hand variables are broken down into all of their levels. Continuous variables are grouped, by default, into quartiles, to summarize the responses. The 'cross' method causes summary.formula to output a data frame containing summary statistics, which is the format in which trellis expects to find raw data. This makes it easy to plot summary statistics using trellis although the summarize function works better for this. method='reverse' reverses the meaning of the left-hand and right-hand-side variables. For example, summary(treatment \sim age + blood.pressure, method='reverse') will print k columns, where k is the number of levels in treatment. For each column, descriptive statistics default to the three quartiles. For categorical ones, frequencies and percentages are computed.

As discussed in Section 3.2.3, nice labels and category levels should have been created early in the process. summary.formula will take full advantage of this.

Here are some of the examples from the online help.

> options(digits=3)

 $^{^{1}}$ Note the inconsistency here: functions such as tapply, aggregate, and by which are built-in to S capitalize the argument into the name FUN.

sex N=500

| | + | + | + | ++ | - |
|-----------|---------|-----|-----|-----|---|
| | I | N | f | m | |
| | + | + | + | ++ | - |
| treatment | Drug | 246 | 123 | 123 | |
| | Placebo | 254 | 129 | 125 | |
| | + | + | + | ++ | - |
| Overall | I | 500 | 252 | 248 | |
| | + | + | + | ++ | - |

> # Compute mean age, separately by sex and treatment > summary(age \sim sex + treatment)

age N=500

| | + | + | ++ |
|-----------|---------|-----|-------------|
| | | | age + |
| | + | | |
| sex | f | 252 | 49.8 |
| | m | 248 | 49.9 |
| | + | + | ++ |
| treatment | Drug | 246 | 49.7 |
| | Placebo | 254 | 50.0 |
| | + | + | ++ |
| Overall | I | 500 | 49.9 |
| | + | + | ++ |

```
> summary(age \sim sex + treatment, method="cross")
Mean of age by sex, treatment
+---+
N I
|age|
+---+
sex|treatment
  |Drug|Plac|ALL |
---+---+
f |123 |129 |252 |
  49.4 50.3 49.8
---+---+
m |123 |125 |248 |
  |50.1|49.7|49.9|
---+---+
ALL 246 254 500
  |49.7|50.0|49.9|
---+---+
> summary(treatment \sim age + sex, method="reverse")
Descriptive Statistics by treatment
-----+
     |Drug |Placebo |
|(N=246) |(N=254) |
----+
age |46.5/49.8/52.5|46.4/50.1/53.4|
-----+
sex : m| 50% (123) | 49% (125) |
-----+
> # a/b/c represents the lower quartile, median, upper quartile
> # Compute predicted probability from a logistic regression model
> # For different stratifications compute receiver operating
> # characteristic curve areas (C-indexes)
> predicted \leftarrow plogis(.4*(sex=="m")+.15*(age-50))
> positive.diagnosis \leftarrow ifelse(runif(500)<=predicted, 1, 0)
> roc \leftarrow function(z) {
+ x \leftarrow z[,1];
+ y \leftarrow z[,2];
+ n \leftarrow length(x);
  if(n<2)return(c(ROC=NA));</pre>
+
+
 n1 \leftarrow sum(y==1);
```

```
+ c(ROC= (mean(rank(x)[y==1])-(n1+1)/2)/(n-n1) );
```

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```
+ }
> y ← cbind(predicted, positive.diagnosis)
> options(digits=2)
```

> summary(y \sim age + sex, fun=roc)

y N=500

| | + | + | ++ |
|---------|--------------|-----|-------|
| | | N | ROC |
| | + | + | ++ |
| age | [32.3,46.4) | 125 | 0.62 |
| | [46.4, 50.0) | 125 | 0.59 |
| | [50.0,52.9) | 125 | 0.61 |
| | [52.9,68.6] | 125 | 0.70 |
| | + | + | ++ |
| sex | f | 252 | 0.71 |
| | m | 248 | 0.70 |
| | + | + | ++ |
| Overall | I | 500 | 0.721 |
| | + | + | ++ |

- > options(digits=3)
- > summary(y \sim age + sex, fun=roc, method="cross")

```
roc by age, sex
+---+
N I
ROC
+---+
        sex
age
       |f |m |ALL |
----+
[32.3,46.4) | 61 | 64 | 125 |
       0.6320.5270.620
----+
[46.4,50.0)| 67 | 58 |125 |
      |0.602|0.671|0.595|
----+
[50.0,52.9) 59 | 66 | 125 |
       0.5170.4450.613
----+
[52.9,68.6] | 65 | 60 | 125 |
     |0.734|0.558|0.703|
----+
ALL
     |252 |248 |500 |
        |0.711|0.702|0.718|
----+
# Plot estimated mean life length (assuming an exponential distribution)
# separately by levels of 4 other variables. Repeat the analysis
# by levels of a column stratification variable, drug. Automatically break
# continuous variables into tertiles (g=3).
# We are using the default, method='response'
life.expect \leftarrow function(y) c(Years=sum(y[,1])/sum(y[,2]))
attach(pbc) # pbc is in UVa biostat web page
S \leftarrow Surv(fu.days/365.25, status)
options(digits=3)
summary(S \sim age + albumin + ascites + edema + stratify(drug),
      fun=life.expect, g=3)
```

Here's an example using the prostate data frame.

```
> detach(2) # detach pbc
> attach(prostate)
> bone ← factor(bm,labels=c("no mets","bone mets"))
> summary(ap ~ sz + bone,
+ fun=function(y) c(Mean=mean(y),quantile(y,c(.25,.5,.75))),
+ method='cross')
c(Mean = mean(y), quantile(y, c(0.25, 0.5, 0.75))) by sz, bone
```

```
+---+
```

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N I Mean |25% | |50% | |75% | +---+ bone SZ |no met|bone m|ALL | -----+ [0,5]|105 | 5 |110 | | 1.0 | 17.7 | 1.8 | |0.40 |2.10 |0.40 | | 0.6 | 3.7 | 0.6 | | 1.00| 38.50| 1.10| ----+ [5,11)|119 | 17 |136 | | 2.2 | 19.1 | 4.4 | |0.40 |1.20 |0.40 | | 0.6 | 1.7 | 0.6 | | 0.85| 9.30| 1.12| ----+ [11,21)|103 | 19 |122 | | 6.5 |139.8 | 27.3 | 0.45 5.30 0.50 | 0.6 | 28.9 | 0.8 | | 1.45|134.14| 3.17| ----+ [21,69] | 88 | 41 | 129 | | 6.3 | 34.8 | 15.4 | |0.60 |4.60 |0.70 | | 1.0 | 20.0 | 2.8 | | 5.67| 35.70| 11.80| ----+ NA 0.50 |0.50 | | 0.7 | | 0.7 | | 1.70| | 1.70| ----+ |420 | 82 |502 | ALL | 3.8 | 54.8 | 12.2 | |0.50 |2.02 |0.50 | | 0.7 | 10.2 | 0.7 | | 1.30| 37.42| 2.97| ----+

| | cscript | we statistics by Treatment | |
|---------------------------------------|---------|---|---|
| | Ν | D-penicillamine $(N = 154)$ | placebo ($N = 158$) |
| Serum Bilirubin (mg/dl) | 418 | 0.725 1.300 3.600 | 0.800 1.400 3.200 |
| Albumin (gm/dl) | 418 | $3.34 \ 3.54 \ 3.78$ | 3.21 3.56 3.83 |
| Histologic Stage, Ludwig Criteria : 1 | 412 | $3\% \frac{4}{154}$ | $8\% \frac{12}{158}$ |
| 2 | | $21\% \frac{32}{154}$ | $22\% \frac{35}{158}$ |
| 3 | | $egin{array}{cccc} 3\% & rac{4}{154} \ 21\% & rac{32}{154} \ 42\% & rac{64}{154} \ 35\% & rac{54}{154} \end{array}$ | $\begin{array}{rrrr} 8\% & \frac{12}{158} \\ 22\% & \frac{35}{158} \\ 35\% & \frac{56}{158} \\ 35\% & \frac{55}{158} \end{array}$ |
| 4 | | $35\% \frac{54}{154}$ | $35\% \frac{55}{158}$ |
| Prothrombin Time (sec.) | 416 | 10.0 10.6 11.4 | 10.0 10.6 11.0 |
| Sex : female | 418 | $90\% \frac{139}{154}$ | $87\% \frac{137}{158}$ |
| Age | 418 | 41.4 48.1 55.8 | 43.0 51.9 58.9 |
| Spiders | 312 | $29\% \frac{45}{154}$ | $28\% \frac{45}{158}$ |

Table 6.1: Descriptive Statistics by Treatment

a b c represent the lower quartile a, the median b, and the upper quartile c for continuous variables. N is the number of non-missing values.

Note that it is possible to get wider column labels using some of summary.formula's options. Also, where you send the output of the function to the Hmisc library's latex function, you get nicely typesetted tables. Here is an example using the latex function (actually latex.default) in conjunction with LATEX. A print method in the Hmisc library for latex objects can be used in this setting for easy on-screen previewing of the typeset table.

The LATEX output is in Table 6.1. The table legend at the bottom was produced by the latex function (actually latex.summary.formula.reverse). If you run the command plot(s), a dot chart will be produced showing the proportions of various categories stratified by drug, and a separate dot chart is drawn for continuous variables. The latter chart shows by default the 3 quartiles of each variable, stratified by drug.

To obtain a comprehensive guide to summary.formula that includes many examples, graphical output, and LATEX commands for putting an entire clinical report together, download the document entitled "Statistical Tables and Plots using S and LATEX" from biostat.mc.vanderbilt.edu/StatReport/summary.pdf. This document also contains graphical representations of may of the example tables. See biostat.mc.vanderbilt.edu/StatReport for useful related material.

6.2.1 Implementing Other Interfaces

The LATEX output can be pasted into a word processed (e.g., Microsoft Word) document in graphics mode if you use PCTEX, with some loss of resolution. A more general solution would be to write S interface functions (e.g., word) that are analogous to the latex family of functions. Such functions would do the needed character string manipulation to write tables and other S output in Word format. It may be easier to implement an S to HTML interface, and Microsoft Word 97 can import HTML files and convert them to Word format. S-PLUS 4.5 and later for Windows has a function html.table for producing simple HTML tables from S matrices. One other possibility is to convert the LATEX code produced by S using a general convertor such as Hevea (see http://www.arch.ohio-state.edu/crp/faculty/pviton/support/hevea.html or http:// biostat.mc.vanderbilt.edu/EmacsLaTeXTools). One problem with this approach is that HTML has some table making features that are not respected by Microsoft Word.

6.3 Graphical Depiction of Two–Way Contingency Tables

The Hmisc symbol.freq function can be used to represent contingency tables graphically. Frequency counts are represented as the heights of "thermometers" by default; you can also specify symbol='circle' to the function. There is an option to include marginal frequencies, which are plotted on a halved scale so as to not overwhelm the plot. Other useful options in this function include orig.scale (set to T when the first two arguments are numeric variables; this uses their original values for x and y coordinates), subset (the usual subsetting argument as used in regression fits), and srtx (a rotation angle for x-axis labels). If you do not ask for marginal frequencies to be plotted using marginals=T, symbol.freq will ask you to click the mouse where a reference symbol is to be drawn to assist in reading the scale of the frequencies. As an example consider

The output is shown in Figure 6.1. See Section 6.1 for ways to display row or column proportions from contingency tables.

Another way to display frequency data is to use the built-in image function to plot the column values vs. the row values, with boxes whose density of shading is a function of the frequency of that cell. To display a two-dimensional histogram for two continuous variables in this way you can run the raw values through the hist2d function.

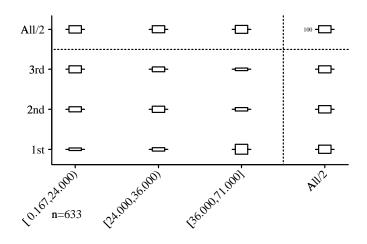


Figure 6.1: A two-way contingency table

Chapter 7

Hmisc Generalized Least Squares Modeling Functions

7.1 Automatically Transforming Predictor and Response Variables

Fitting multiple regression models by the method of least squares is one of the most commonly used methods in statistics. There are a number of challenges to the use of least squares, even when it is only used for estimation and not inference, for example:

- 1. How should continuous predictors be transformed so as to get a good fit?
- 2. Is it better to transform the response variable? How does one find a good transformation that simplifies the right hand side of the equation?
- 3. What if Y needs to be transformed non-monotonicially (e.g., |Y 100| or $(Y 120)^2$) before it will have any correlation with X?

When one is trying to draw inference about population effects using confidence limits or hypothesis tests, the most common approach is to assume that the residuals have a normal distribution. This is equivalent to assuming that the conditional distribution of the response Y given the set of predictors X is normal with mean depending on X and variance that is (hopefully) a constant independent of X. The need for a distributional assumption to enable us to draw inferences creates a number of other challenges, including:

1. If for the untransformed original scale of the response Y the distribution of the residuals is not normal with constant spread, ordinary methods will not yield correct inferences (e.g., confidence intervals will not have the desired coverage probability and the intervals will need to be asymmetric).

- 2. Quite often there is a transformation of Y that will yield well-behaving residuals. How do you find this transformation? Can you find transformation for the Xs at the same time?
- 3. All classical statistical inferential methods assume that the full model was pre–specified, i.e., the model was not modified after examining the data. How does one correct confidence limits, for example, for data–based model selection?

On the last point, Faraway [15] demonstrated that the more stops done by the analyst, such as looking for transformations, outliers, overly influential observations, and stepwise variable selection, the more the variance of estimates increases. This assumes of course that one properly estimates the variances (e.g., using a simulation technique such as the bootstrap); *apparent* variances will typically *decrease* as the model is refined. Faraway showed that the greatest source of inflation of actual variances is letting the data dictate the transformation of Y. He concluded that since we currently have no statistical theory for deriving proper variance estimates, it is preferable to automate the analysis and to use the bootstrap to estimate variances and construct confidence limits, taking into account all sources of variability induced by the modeling strategy.

S has a powerful function, gam, for fitting generalized additive regression models. gam automatically estimates the transformation each right hand side variable should receive so as to optimize prediction of Y, and a number of distributions are allowed for Y. When one hopes to assume normality and the left hand side of the model also needs transformation, either to improve R^2 or to achieve constant variance of the residuals (which increases the chances of satisfying the normality assumption), S has two powerful nonparametric regression functions: ace and avas. Both functions allow categorical predictors, allow predictor transformations to be non-monotonic, and allow the analyst to restrict the transformations to be monotonic. ace stands for "alternating conditional expectation" [16], an algorithm directed solely at finding transformations for all variables simultaneously so as to optimize R^2 . ace will allow Y to be non-monotonically transformed, and it is based on the "super smoother" (see the supsmu function). avas stands for "additivity and variance stabilization" [17]. avas tries to maximize R^2 while forcing the transformation for Y to result in nearly constant variance of residuals. avas restricts the transformation of Y to be monotonic.

ace and avas are quite powerful, but they can result in overfitting, and they provide no statistical inferential measures. In addition, they do not use the S modeling language, so they are slightly more difficult to use. The Hmisc areg.boot ("additive regression using the bootstrap") solves these problems. The bootstrap is used to estimate the optimism (bias) in the apparent R^2 , and this optimism is subtracted from the apparent R^2 to get a more trustworthy estimate. The online help file has the details.

Note: areg.boot has been extended to allow one to estimate any quantity of interest, such as the mean response, on the original scale, using Duan's smearing estimator. The output below is from the previous version of areg.boot which did not include this facility. See Chapter 15 of Harrell's book REGRESSION MODELING STRATEGIES for an updated example.

As an example consider an excellent dataset provided by Dr. John Schorling, Department of Medicine, University of Virginia School of Medicine. The data consist of 19 variables on 403 subjects from 1046 subjects who were interviewed in a study to understand the prevalence of obesity and diabetes in central Virginia for African Americans. According to Dr. John Hong, Diabetes Mellitus Type II (adult onset diabetes) is associated most strongly with obesity. The waist/hip ratio may be a predictor of diabetes and heart disease. DM II is also associated with hypertension - they may both be part of "Syndrome X". The 403 subjects were the ones who were actually screened for diabetes. Glycosolated hemoglobin > 7.0 is usually taken as a positive diagnosis of diabetes.

7.1. AUTOMATICALLY TRANSFORMING PREDICTOR AND RESPONSE VARIABLES 155

At first glance some analysts might think that the best way to develop a model for diagnosing diabetes might be to fit a binary logistic model with glycosolated hemoglobin > 7 as the response variable. This is very wasteful of information, as it does not distinguish a hemoglobin value of 2 from a 6.9, or a 7.1 from a 10. The waste of information will result larger standard errors of $\hat{\beta}$, wider confidence bands, larger *P*-values, and lower power to detect risk factors. A better approach is to predict the continuous hemoglobin value using a continuous response model such as ordinary multiple regression or using ordinal logistic regression. Then this model can be converted to predict the probability that hemoglobin exceeds any cutoff of interest. For an ordinal logistic model having one intercept per possible value of hemoglobin in the dataset (except for the lowest value), all probabilities are easy to compute. For ordinary regression this probability depends on the distribution of the residuals from the model.

Let us proceed with a least squares approach. An initial series of trial transformations for the response indicated that the reciprocal of glycosolated hemoglobin resulted in a model having residuals of nearly constant spread when plotted against predicted values. In addition, the residuals appeared well approximated by a normal distribution. On the other hand, a model developed on the original scale did not have constant spread of the residuals. It will be interesting to see if the nonparametric variance stabilizing function determined by **avas** will resemble the reciprocal of hemoglobin.

Let's consider the following predictors: age, systolic blood pressure, total cholesterol, body frame (small, medium, large), weight, and hip circumference. 12 subjects have missing body frame, and we should be able to impute this variable from other body size measurements. Let's do this using recursive partitioning with Atkinson and Therneau's **rpart** function. See the UVa Web page for a link to obtain the **rpart** library. The advantage of **rpart** over the builtin **tree** function is that **rpart** can handle missing predictor variables using "surrogate splits." In other words, when a predictor needed for classifying an observation is missing, other predictors that are not missing can be used as stand-ins. **rpart** will predict the probability that the polytomous response **frame** equals each of its three levels.

```
> library(rpart)
> r \leftarrow rpart(frame \sim gender + height + weight + waist + hip)
> plot(r); text(r) # shows first split on waist, then height, weight
> probs <- predict(r, diabetes)
> # Within each row of probs order from largest to smallest
> # Find column # of largest
> most.probable.category \leftarrow (t(apply(-probs, 1, order)))[,1]
> frame.pred ~ levels(frame)[most.probable.category]
> table(frame, frame.pred)
       large medium small
 small
           2
                 45
                        57
medium
          10
                158
                        16
          35
                 67
                         1
 large
> frame ~ impute(frame, frame.pred[is.na(frame)])
> describe(frame)
frame : Body Frame
   n missing imputed unique
 403
           0
                   12
                           3
```

Other predictors are only missing on a handful of cases. Impute them with constants to avoid excluding any observations from the fit.

Now fit the **avas** model. Do only 30 bootstrap repetitions so we can clearly see how the bootstrap re-estimates of transformations vary on the next plot. Use subject matter knowledge to restrict the transformations of **age**, weight, and hip to be monotonic. Had we wanted to restrict transformations to be linear, we would have specified the identity function, e.g., I(weight).

```
> f ← areg.boot(glyhb ~ monotone(age) + bp.1s + chol + frame +
+ monotone(weight) + monotone(hip), B=30)
> options(digits=3)
> f
avas Additive Regression Model
areg.boot(x = glyhb ~ monotone(age) + bp.1s + chol + frame +
monotone(weight) + monotone(hip), B = 30)
Categorical variables: frame
```

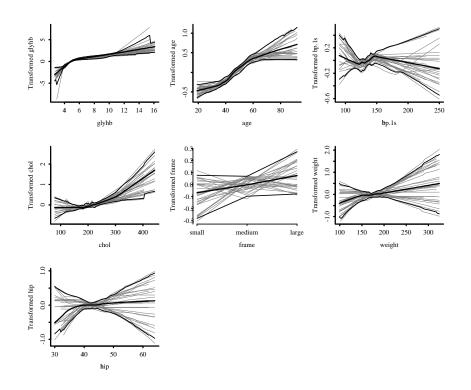


Figure 7.1: avas transformations: overall estimates, pointwise 0.95 confidence bands, and 30 bootstrap estimates.

Frequencies of Missing Values Due to Each Variable glyhb monotone(age) bp.1s chol frame monotone(weight) monotone(hip) 13 0 0 0 0 0 0 n= 390 p= 6 Apparent R2 on transformed Y scale: 0.265 Bootstrap validated R2 : 0.207 Coefficients of standardized transformations: Intercept age bp.1s chol frame weight hip -4.34e-009 1.06 1.51 0.953 0.708 1.26 0.653

Note that the coefficients above do not mean very much as the scale of the transformations is arbitrary. We see that the model was overfit a moderate amount (optimism in R^2 is 0.265 - 0.207).

Next we plot the transformations (bold lines in the center), pointwise 0.95 confidence bands (shown with bold lines), and bootstrap estimates (smaller lines).

> plot(f, col.boot=.75) # use grayscale instead of color for bootstraps

The plot is shown in Figure 7.1. Apparently, age and chol are the important predictor.

Let's see how effective the transformation of glyhb was in stabilizing variance and making the residuals normally distributed.

```
> par(mfrow=c(2,2))
> plot(fitted(f), resid(f))
> plot(predict(f), resid(f))
> qqnorm(resid(f)); abline(a=0, b=1) # draws line of identity
```

We see from Figure 7.2 that the residuals have reasonably uniform spread and are distributed almost normally. A multiple regression run on untransformed variables did not fare nearly as well.

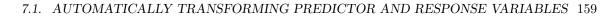
Now check whether the response transformation is close to the reciprocal of glyhb. First derive an S representation of the fitted transformations. For nonparametric function estimates these are really table lookups. Function creates a list of functions, named according to the variables in the model.

```
> funs ~ Function(f)
> plot(1/glyhb, funs$glyhb(glyhb))
```

Results are in Figure 7.3. An almost linear relationship is evidence that the reciprocal is a good transformation¹.

Now let's get approximate tests of effects of each predictor. summary does this by setting all other predictors to reference values (e.g., medians), and comparing predicted untransformed responses for a given level of the predictor with predictions for the lowest setting of X. We will use the three quartiles for continuous variables, but specify **age** settings manually.

¹Beware that it may not help to know this, because if we re-do the analysis using an ordinary linear model on 1/glyhb, standard errors would not take model selection into account[15].



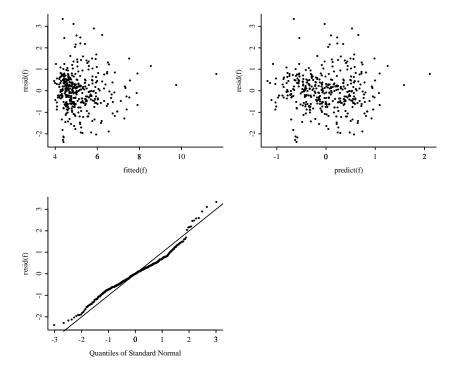


Figure 7.2: Distribution of residuals from the **avas** fit. The top left panel x-axis has \hat{Y} on the original Y scale. The top right panel uses the transformed \hat{Y} for the x-axis.

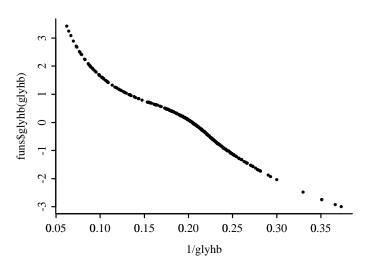


Figure 7.3: Agreement between the avas transformation for glyhb and the reciprocal of glyhb.

> summary(f, values=list(age=c(20,30,40,50,60,70,80)))

Values to which predictors are set when estimating effects of other predictors:

glyhb age bp.1s chol frame weight hip 4.84 50 136 204 2 173 42

Estimates of differences of effects on Y (from first X value), and bootstrap standard errors of these differences. Settings for X are shown as row headings.

| Predic | ctor: age | | | | | |
|--------|-----------|--------|------------|------------|------|-----------|
| Dif | fferences | S.E | Lower 0.95 | Upper 0.95 | Z | Pr(Z) |
| 20 | 0.000 | NA | NA | NA | NA | NA |
| 30 | 0.064 | 0.0434 | -0.0210 | 0.149 | 1.48 | 1.40e-001 |
| 40 | 0.184 | 0.0770 | 0.0326 | 0.335 | 2.38 | 1.72e-002 |
| 50 | 0.527 | 0.1084 | 0.3149 | 0.740 | 4.87 | 1.14e-006 |
| 60 | 0.868 | 0.1551 | 0.5645 | 1.172 | 5.60 | 2.14e-008 |
| 70 | 1.122 | 0.2311 | 0.6691 | 1.575 | 4.86 | 1.20e-006 |
| 80 | 1.428 | 0.4591 | 0.5278 | 2.327 | 3.11 | 1.87e-003 |

| Predictor: bp.1s | | | | | | | |
|------------------|-------------|--------|------------|------------|------|---------|--|
| | Differences | S.E | Lower 0.95 | Upper 0.95 | Z | Pr(Z) | |
| 122 | 0.0000 | NA | NA | NA | NA | NA | |
| 136 | 0.0863 | 0.0715 | -0.0540 | 0.227 | 1.21 | 0.2279 | |
| 148 | 0.2275 | 0.1303 | -0.0278 | 0.483 | 1.75 | 0.0807 | |

| Pre | dictor: chol | | | | | |
|-----|--------------|--------|------------|------------|------|---------|
| | Differences | S.E | Lower 0.95 | Upper 0.95 | Z | Pr(Z) |
| 179 | 0.0000 | NA | NA | NA | NA | NA |
| 204 | 0.0715 | 0.0606 | -0.0473 | 0.190 | 1.18 | 0.2381 |
| 229 | 0.1912 | 0.1111 | -0.0265 | 0.409 | 1.72 | 0.0852 |

| Predictor: frame | | | | | | | |
|------------------|-------------|-------|-------|-------|------------|-------|---------|
| | Differences | S.E | Lower | 0.95 | Upper 0.95 | Z | Pr(Z) |
| small | 0.0000 | NA | | NA | NA | NA | NA |
| medium | 0.0514 | 0.119 | -(|).182 | 0.285 | 0.433 | 0.665 |
| large | 0.1141 | 0.176 | -(| 0.231 | 0.459 | 0.648 | 0.517 |

| Predictor: weight | | | | | | | |
|-------------------|-------------|-------|------------|------------|-------|---------|--|
| | Differences | S.E | Lower 0.95 | Upper 0.95 | Z | Pr(Z) | |
| 150 | 0.0000 | NA | NA | NA | NA | NA | |
| 173 | 0.0219 | 0.109 | -0.192 | 0.236 | 0.201 | 0.841 | |
| 200 | 0.1576 | 0.245 | -0.322 | 0.637 | 0.644 | 0.520 | |

Predictor: hip Differences S.E Lower 0.95 Upper 0.95 Z Pr(|Z|)NA NA 39 O.OOOO NA NA NA 0.0097 0.102 -0.189 0.209 0.0955 42 0.924 46 0.0299 0.200 -0.362 0.422 0.1496 0.881 Warning messages: For 5 bootstrap samples a predicted value for one of the settings for age could not be computed. These bootstrap samples ignored. Consider using less extreme predictor settings. in: summary.areg.boot(f, values = list(age = c(20, 30, 40, 50, 60, 70, 80)))

For example, when age increases from 20 to 70 we predict an increast in glyhb by 1.122 with standard error 0.2311, when all other predictors are help to constants listed above. Setting them to other constants will yield different estimates of the age effect, as the transformation of glyhb is nonlinear. We see that only for age do some of the confidence intervals for effects exclude zero.

Let's depict the fitted model by plotting predicted values, with age varying on the x-axis, and 3 curves corresponding to three values of chol. Set all other predictors to representative values.

The result is Figure 7.4. Note that none of the predictions is above 7.0. Let's see how many predictions in the entire dataset are above 7.0.

So the model is not very useful for finding clinical levels of diabetes. Let's make sure that a dedicated binary model would not do any better.

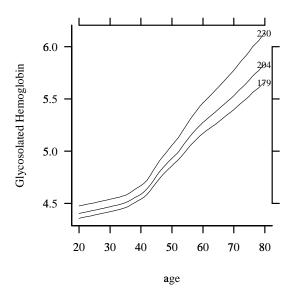


Figure 7.4: Predicted median glyhb as a function of age and chol.

Logistic Regression Model

```
lrm(formula = glyhb > 7 \sim rcs(age, 4) + rcs(bp.1s, 3) +
   rcs(chol, 3) + frame + rcs(weight, 4) + rcs(hip, 3))
Frequencies of Responses
FALSE TRUE
  330
        60
Frequencies of Missing Values Due to Each Variable
glyhb > 7 age bp.1s chol frame weight hip
       13
            0
                  0
                       0
                             0
                                    0
                                       0
                                   C Dxy Gamma Tau-a R2 Brier
Obs Max Deriv Model L.R. d.f. P
390
       1e-007
                    71.3
                          14 0 0.819 0.637 0.639 0.166 0.29 0.105
                  Coef
                          S.E. Wald Z
                                           Ρ
  Intercept -16.804027 6.40143 -2.63 0.0087
              0.023219 0.08806 0.26
                                      0.7920
        age
       age'
              0.266699 0.25501 1.05
                                      0.2956
      age'' -0.852166 0.63708 -1.34 0.1810
      bp.1s
             0.028259 0.02476 1.14 0.2537
     bp.1s' -0.025207 0.02404 -1.05
                                      0.2944
       chol
             0.004649 0.01004 0.46 0.6432
      chol'
              0.003535 0.01046 0.34 0.7354
frame=medium -0.246480 0.48146 -0.51 0.6087
frame=large -0.266503 0.53384 -0.50 0.6176
```

| weight | 0.042962 | 0.03073 | 1.40 | 0.1621 |
|----------|-----------|---------|-------|--------|
| weight' | -0.088281 | 0.09463 | -0.93 | 0.3509 |
| weight'' | 0.264845 | 0.29109 | 0.91 | 0.3629 |
| hip | 0.033904 | 0.12479 | 0.27 | 0.7859 |
| hip' | -0.053349 | 0.13979 | -0.38 | 0.7027 |
| | | | | |

| > anova(h) | | | | | | |
|-----------------|----------------|------|-----------|-------|---|---|
| Wa | ald Statistics | | Response: | glyhb | > | 7 |
| | | | | | | |
| Factor | Chi-Square | d.f. | Р | | | |
| age | 23.85 | 3 | 0.0000 | | | |
| Nonlinear | 6.82 | 2 | 0.0331 | | | |
| bp.1s | 1.32 | 2 | 0.5178 | | | |
| Nonlinear | 1.10 | 1 | 0.2944 | | | |
| chol | 5.45 | 2 | 0.0657 | | | |
| Nonlinear | 0.11 | 1 | 0.7354 | | | |
| frame | 0.29 | 2 | 0.8630 | | | |
| weight | 5.41 | 3 | 0.1443 | | | |
| Nonlinear | 0.87 | 2 | 0.6457 | | | |
| hip | 0.19 | 2 | 0.9111 | | | |
| Nonlinear | 0.15 | 1 | 0.7027 | | | |
| TOTAL NONLINEAR | 10.48 | 7 | 0.1630 | | | |
| TOTAL | 45.65 | 14 | 0.0000 | | | |

So far the results seem to be the same as using a continuous response. How many predicted probabilities of diabetes are in the "rule–in" range?

Only one patient had a predicted probability > 0.8. So the risk factors are just not very strong, although age does explain some pre-clinical variation in glyhb.

7.2 Robust Serial Data Models: Time– and Dose–Response Profiles

Serial data (repeated measurements) are commonly encountered in biostatistical analysis. Specialized methods exist for fitted repeated measurements but it is advantageous to fit time– and dose–response data using a flexible parametric approach while allowing calculation of simultaneous (and pointwise) confidence limits for the true trends. The approach taken by Hmisc's **rm.boot** function is to use a "working independence" model allowing for intercepts to vary by subjects, and then to account for intra–subject correlations when deriving confidence bands. Regression splines restricted to be linear beyond the outer join points (knots) are used to fit the overall trend. Here all the serial data are analyzed in a common model with dummy variables used to absorb subject effects. Regression estimates which do not take the correlation structure into account are often quite efficient. Then a cluster bootstrap (sampling with replacement from *subjects* rather than data points) [18] is used to compute confidence bands in a nearly nonparametric fashion. The text below, taken from the help file for rm.boot, describes the details. In what follows, "time" can be replaced with other variables such as the dose of a drug given multiple times to the same subjects.

For a dataset containing a time variable, a scalar response variable, and an optional subject identification variable, rm.boot obtains least squares estimates of the coefficients of a restricted cubic spline function or a linear regression in time after adjusting for subject effects through the use of subject dummy variables. Then the fit is bootstrapped B times, either by treating time and subject id as fixed (i.e., conditioning the analysis on them) or as random variables. For the former, the residuals from the original model fit are used as the basis of the bootstrap distribution. For the latter, samples are taken jointly from the time, subject id, and response vectors to obtain unconditional distributions.

If a subject id variable is given, the bootstrap sampling will be based on samples with replacement from subjects rather than from individual data points. In other words, either none or all of a given subject's data will appear in a bootstrap sample. This cluster sampling takes into account any correlation structure that might exist within subjects, so that confidence limits are nonparametrically corrected for within-subject correlation. Assuming that ordinary least squares estimates, which ignore the correlation structure, are consistent (which is almost always true) and efficient (which would not be true for certain correlation structures or for datasets in which the number of observation times vary greatly from subject to subject), the resulting analysis will be a robust, efficient repeated measures analysis for the one-sample problem.

Predicted values of the fitted models are evaluated by default at a grid of 100 equally spaced time points ranging from the minimum to maximum observed time points. Predictions are for the average subject effect. Pointwise confidence intervals are optionally computed separately for each of the points on the time grid. However, simultaneous confidence regions that control the level of confidence for the entire regression curve lying within a band are often more appropriate, as they allow the analyst to draw conclusions about nuances in the mean time response profile that were not stated apriori. The method of Tibshirani and Knight [19] is used to easily obtain simultaneous confidence sets for the set of coefficients of the spline or linear regression function as well as the average intercept parameter (over subjects). Here one computes the objective criterion (here both the -2 log likelihood evaluated at the bootstrap estimate of beta but with respect to the original design matrix and response vector, and the sum of squared errors in predicting the original response vector) for the original fit as well as for all of the bootstrap fits. The confidence set of the regression coefficients is the set of all coefficients that are associated with objective function values that are less than or equal to say the 0.95 quantile of the vector of B + 1 objective function values. For the coefficients satisfying this condition, predicted curves are computed at the time grid, and minima and maxima of these curves are computed separately at each time point to derive the final simultaneous confidence band.

By default, the log likelihoods that are computed for obtaining the simultaneous confidence band assume independence within subject. This will cause problems unless such log likelihoods have very high rank correlation with the log likelihood allowing for dependence. To allow for correlation or to estimate the correlation function, see the cor.pattern and rho arguments to rm.boot.

As most repeated measurement studies consider the times as design points, the fixed covariable case is the default. Bootstrapping the residuals from the initial fit assumes that the model is correctly specified. Even if the covariables are fixed, doing an unconditional bootstrap is still appropriate, and for moderate to large sample sizes unconditional confidence intervals are only slightly wider than conditional ones if subject effects (intercepts) are small. For bootstrap.type="x random" in the

presence of significant subject effects, the analysis is approximate as the subjects used in any one bootstrap fit will not be the entire list of subjects. The average (over subjects used in the bootstrap sample) intercept is used from that bootstrap sample as a predictor of average subject effects in the overall sample.

rm.boot can handle two-sample problems in which trends are fitted separately within each of two groups and then the differences in the trends (and bootstrap confidence bands for these) are computed to measure the group effect.

7.2.1Example

The following example demonstrates how correlated response data may be simulated and then analyzed using rm.boot. We simulate data for 20 subjects each with 11 response measurements. The population response function is piecewise linear (flat in the left and right tails) and large true subject effects are present.

```
store()
# Don't keep any of the objects created (store is in Hmisc)
# Function to generate n p-variate normal variates with
# mean vector u and covariance matrix S
# Slight modification of function written by Bill Venables
\texttt{mvrnorm} \leftarrow \texttt{function}(\texttt{n, p = 1, u = rep(0, p), S = diag(p))} \{
  Z \leftarrow matrix(rnorm(n * p), p, n)
  t(u + t(chol(S)) %*% Z)
# Simulate serial data
      ← 20
                      # Number of subjects
n
sub
      \leftarrow .5*(1:n)
                      # Subject effects
# Specify functional form for time trend and compute
# non-stochastic component
times \leftarrow seq(0, 1, by=.1)
      \leftarrow function(times) 5*pmax(abs(times-.5),.3)
g
      \leftarrow g(times)
ev
# Generate multivariate normal errors for 20 subjects at 11 times
# Assume equal correlations of rho=.7, independent subjects
      \leftarrow length(times)
nt
rho
      \leftarrow .7
set.seed(19)
errors \leftarrow mvrnorm(n, p=nt, S=diag(rep(1-rho,nt))+rho)
# Note: first random number seed used gave rise to
# mean(errors)=0.24!
```

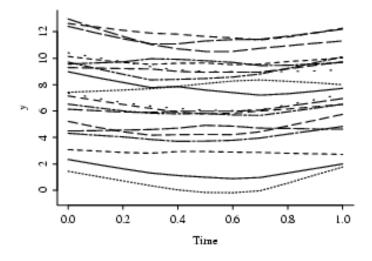


Figure 7.5: Nonparametric estimates of time trends for individual subjects

```
# Add E[Y], error components, and subject effects
y
       ← matrix(rep(ey,n), ncol=nt, byrow=T) + errors +
          matrix(rep(sub,nt), ncol=nt)
# String out data into long vectors for times, responses,
# and subject ID
       \leftarrow as.vector(t(y))
у
times
       \leftarrow rep(times, n)
       \leftarrow sort(rep(1:n, nt))
id
# Do 400 bootstrap repetitions, sampling from residuals (grouped by
# subjects) rather than from the design matrix and responses for
# subjects
f \leftarrow rm.boot(times, y, id, plot.individual=T, B=400,
```

To compute a dependent-structure log-likelihood in addition to one assuming independence, add e.g. the argument cor.pattern='estimate' or rho=.5.

smoother=lowess, bootstrap.type='x fixed', nk=6)

plot.individual=T, smoother=lowess causes nonparametric estimates of trends for individual subjects to be plotted on a single plot. The output from this object is shown in Figure 7.5.

Next we plot a random sample of 75 of the 400 bootstrap fits of the time trends. These fits use as intercepts the average intercept over subjects.

```
plot(f, individual.boot=T, ncurves=75, ylim=c(6,8.5))
```

The plot is in Figure 7.6.

Finally the main plot of interest is shown in Figure 7.7. Both simultaneous and pointwise confidence regions are shown.

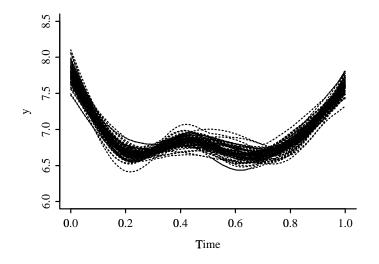


Figure 7.6: 75 of the 400 bootstrap estimates of the average time trend over subjects.

plot(f, pointwise.band=T, col.pointwise=1, ylim=c(6,8.5))

rm.boot assumes that any missing measurements are missing completely at random. The Design rm.impute function can analyze non-randomly missing serial data using multiple imputation, assuming that the probability that a measurement is missing is a function only of baseline variables and of previous measurements.

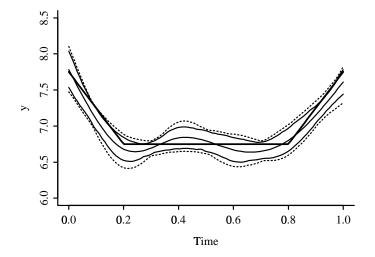


Figure 7.7: Simultaneous (dotted outer curves) and pointwise (solid curves) 0.95 confidence regions for the average time trend. The plot also has the overall fitted time trend as the solid curve in the middle, and the true piecewise linear population time trend for the true average subject effect. The confidence intervals assume that a restricted cubic spline function with 6 knots contains the population profile as a special case, which is not exactly true.

Chapter 8

Builtin S Functions for Multiple Linear Regression

lm is the builtin function for fitting multiple linear regression models, and it works with several other functions to summarize results, make hypothesis tests, get predicted values, and display model diagnostics. Suppose that the response variable is named y and the predictors are x1, x2, x3. The following examples show how to use the basic functions. Note that the *fit object* below (f) is a list containing several components such as coefficients and fitted.values.

```
# Use the following command to cause dummy variables to be created
# the conventional way from categorical predictors
options(contrasts=c('contr.treatment','contr.poly'))
# Fitting functions in the Design library make this the default
f \leftarrow lm(y \sim x1 + x2 + x3, data=dframe, na.action=na.omit)
# Attach dframe if you don't use data=, omit both if using
# standalone variables
# Omit na.action= if there are no NAs in the variables in the model
# na.omit causes any observations containing NAs to be deleted
# before fitting
f
            # or print(f): prints coefficients and sigma hat
summary(f) # prints crude residual diagnostics, coefficients,
            # s.e., t statistics, P-values, sigma hat, overall F and P,
            # R^2, correlations of coefficients
plot(f)
            # Draws 6 graphs
# Plots residuals vs. fitted values (with 3 most extreme
# points identified),
# sqrt(abs(residuals)) vs. yhat (for identifying outliers)
```

```
# y vs. yhat
# normal quantile plot of residuals (to check for normality)
# a residual-fit spread plot (r-f plot) to compare the spread of the
# fitted values with the spread of residuals (which should be less)
# Cook's distance plot to look for overly influential observations
plot(f, smooths=T, rugplot=T)
# adds trend lines and x data density ticks
coef(f)
           # or coefficients(f) or f$coefficients: get coef.
fitted(f) # or fitted.values(f) or predict(f) or
           # f$fitted.values: computes yhat
           # or residuals(f) or f$residuals: computes residuals
resid(f)
plot(x2, resid(f)) # plot residuals vs. x2 alone
predict(f, se.fit=T)
# original hats and se for E(y|x)
predict(f, data.frame(x1=1,x2=2,x3=17))
# yhat for user-given x's
predict(f, expand.grid(x1=1,x2=2:3,x3=1:10))
# yhat for 20 combinations of x's
# Use e.g. sex=factor('female',levels=...) to specify settings of
# categorical predictors
           # compute SSR due to each variable by
drop1(f)
           # dropping one at a time
aov(f)
           # sums of squares and d.f.
anova(f)
           # anova table with sums of squares computed by
           # sequentially adding predictors (in order in formula),
           # F, P-values
f2 \leftarrow lm(y \sim x3)
                     # sub-model
anova(f2, f)
                    # partial F test for x1+x2 combined | x3 plus
                    # sequentially added sums of squares
# To get partial F tests for all variables, you must leave out each
# at a time
# Without controlling x2 and x3, plot yhat vs. observed x1 with
# pointwise 0.99 CI
pred \leftarrow predict(f, se.fit=T)
plot(x1, fitted(f))
points(x1, ci$upper, pch=2)
points(x1, ci$lower, pch=2)
# Better:
# Let x1 vary over a grid of 100 equally spaced points and set
# x2 and x3 to their means. Get predicted values and s.e., then
```

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```
# pass predictions through pointwise() to get pointwise CI to plot
x1s \leftarrow seq(min(x1),max(x1), length=100)
pred \leftarrow predict(f, expand.grid(x1=x1s, x2=mean(x2), x3=mean(x3)),
              se.fit=T)
pred$fit
             # print yhat
            # print estimated se of yhat
pred$se.fit
ci ← pointwise(pred, coverage=.95)
ci$upper
             # print upper CL
ci$lower
             # print lower CL
plot(x1s, pred$fit, type='l', ylab='Yhat')
lines(x1s, ci$upper, lty=2)
                            # dotted line
lines(x1s, ci$lower, lty=2)
# Add confidence bands for predicting individual y's
# pred$residual.scale^2 is MSE, and this is for the '1'
# in the se(E(y|x)) formula
cii ← pointwise(pred, coverage=.95)
lines(x1s, cii$lower, lty=2)
lines(x1s, cii$upper, lty=2)
# An example where we get predictions by letting two predictors
# vary, and we plot two sets of confidence bands
ages \leftarrow seq(3,16,length=100)
pred
      ← predict(fit, combos, se.fit=T)
ci
      ← pointwise(pred, coverage=.99)
par(mfrow=c(1,2))
for(sx in levels(sex)) {
  s \leftarrow combos
  plot(combos$age[s], ci$fit[s], xlab='Age', ylab='Y hat',
       ylim=range(unlist(ci)), type='l')
  # range(unlist(ci)) takes range over all of fit, upper, lower
  title(sx)
  lines(combos$age[s], ci$upper[s], lty=2)
  lines(combos$age[s], ci$lower[s], lty=2)
}
```

To obtain partial residual plots you can use the Statistics .. Regression .. Linear menu in version 4.0 and later.

Warning: When the response or any of the predictor variables contain NAs, na.action=na.omit will cause lm to delete observations containing NAs, but unfortunately the fitted, resid, and predict (when no data frame argument is given) functions compute \hat{y} or residuals only for the observations actually used in the fit. In other words, the results of these functions will be vectors that are shorter than the original variables used in the fit, and the observations will no longer align. A command such as plot(x1, resid(fit)) will fail. One solution to the problem is to attach only the subset of the data frame that corresponds to observations not containing NAs on variables used in modeling. This approach does not work well when different sets of variables are to be used in different models. The survival analysis modeling functions builtin to S solve this problem in an elegant way. Regression fitting functions (such as ols) in the Design library use this same solution. These fitting functions set up so that resid and related functions add NAs back to predicted values or residuals so that they are aligned with the original data.

Warning: When the 1m model contains a categorical (factor) predictor, you must give predict a data frame that has exactly the same factor levels for such predictors as appeared in the original variable given to 1m. For example, specifying predict(fit, data.frame(age=10, sex='male')) can result in incorrect predictions, as the temporary sex variable contains only one level, and predict for 1m does not know how to construct the dummy variables correctly. Instead, specify for example

if the original sex variable had levels c('female', 'male') in that order. A more automatic approach is to specify sex=factor('male', levels(sex)) in the previous command. To obtain predictions for all values of a categorical predictor, use for example sex=factor(c('male', 'female'), levels(sex)) or sex=factor(levels(sex), levels(sex)) as in one of the examples above.

All fitting functions in the **Design** library solve this problem by looking up the original **levels** for all predictors. No other S functions handle this automatically.

When using lm instead of Design's ols function, you may want to put the contrasts option in your .First function, e.g.:

```
.First ← function() {
    library(Hmisc,T)
    options(contrasts=c('contr.treatment','contr.poly'))
  }
```

8.1 Sequential and Partial Sums of Squares and *F*-tests

Sequential sums of squares (called Type I SS in SAS) are increments in SSR's as predictors are added to a model¹. Sequential SS can be quite arbitrary, because the SS for all predictors depend on the order that predictors were listed in the model formula. Sequential F-statistics are defined as sequential mean squares divided by the MSE from the full model. These statistics test the hypothesis that the current predictor is associated with the response after adjusted for the list of predictors that preceded it. In other words, a sequential F-test tests whether the current predictor adds predictive information to those listed before it. Only the last predictor's sequential SS is adjusted for all of the other predictors. The total of all the sequential SS equals the SSR for the entire model.

In S, sequential *F*-tests are obtained by the command anova(fitobject).

Partial sums of squares (called Type II, III, or IV SS in SAS^2) are increments in SSR's when each predictor is added to all of the other predictors. Partial F-statistics are partial mean squares divided by the MSE. A partial test tests whether the current predictor is associated with the response after adjustment for all other predictors. In other words, the partial test assesses whether

¹Note that increments in SSR are decrements in SSE. SSE is called RSS (residual sums of squares) in Rosner. ²These three types are identical when there are no interactions involving the predictors being tested

the predictor adds information to all of the other predictors. The sequential SS for the last predictor in a model equals its partial SS. The total of all partial SS does not mean anything.

Recall that the regression coefficients are also called partial regression coefficients, and that all of the *t*-statistics that are printed with the model fit (by e.g., summary(fit)) are test statistics for testing partial effects. When a predictor has only one degree of freedom associated with it (i.e., it is represented by one regression coefficient), its partial *F*-statistic is the square of the *t*-statistic (obtained by dividing the coefficient estimate by its estimated standard error).

Partial *F*-tests for multiple degree of freedom predictors are obtained in S by fitting a sub-model in which the predictor of interest is deleted, and then issuing a command such as **anova(fit.submodel,fit.full)**. The difference in *SSR*'s for the full and reduced models the partial *SS* for the omitted predictor. The partial test thus assesses how much predictive information is lost by deleting that predictor.

Consider the following table of sequential and partial SS for a model containing predictors age, sex, and exposure (in that order):

| Predictor | Sequential SS | Partial SS |
|-----------|-----------------|--------------|
| Age | 1000 | 755 |
| Sex | 300 | 100 |
| Exposure | 5 | 5 |
| Total | 1305 | |

As exposure is listed last, its sequential SS equals its partial SS. If the order of variables were to be reversed, we might see the following table:

| Predictor | Sequential SS | Partial SS |
|----------------|-----------------|--------------|
| Exposure | 150 | 5 |
| \mathbf{Sex} | 400 | 100 |
| Age | 755 | 755 |
| Total | 1305 | |

Now we see that if age and sex are not adjusted for, exposure explains more of the variation in the response. In contrast, exposure adds only 5 to SSR once age and sex are held constant. sex adds 100 more to SSR when only exposure is adjusted for, compared to when only age is adjusted for.

The easiest way to get partial F-tests and P-values for predictors that have one parameter associated with them is to use the partial t-tests that are printed by the S summary command (you can square t to get F). The easiest way to partial SS and F-tests in general is to run the **anova** function on a model that has the variable of interest as the last variable in the model, e.g.:

anova(lm(y \sim age + sex + cholesterol))

This will give an unadjusted test for age, a fully adjusted (partial) test for cholesterol, and a test for sex that is only adjusted for age. S-PLUS 4.5 and later has extended the anova function to compute all partial tests using Type III sums of squares³. To obtain these partial tests, use the command anova(fit,ssType=3). Type III tests are problematic, however, when interactions are present in the model — just the situation where Type III F-tests were originally intended to have advantages. For example, in a multi-center randomized drug trial for which treatment × center interactions are included in the model, Type III tests for the "average" drug effect weight

³The anova command for the Design library prints all partial F or χ^2 tests automatically.

centers contributing very few patients the same as large centers. The weighted mean (over centers) treatment effect associated with the Type III test is strange indeed, as it is a simple unweighted average of center–specific treatment effects and thus has lower precision.

For pre–4.5 versions of S-PLUS the shortest command for obtaining a general pooled partial F-test is

anova(lm(y \sim subset of variables), lm(y \sim full set of variables))

where the subset of variables is the set of variables aside from the ones being tested. For the Design library, you can just list the variables you want to combine in an **anova** command.

Sometimes the order of variables can result in meaningful sequential SS for all variables. For example, one might list patient measurements in the order of the cost of making the measurements. Then each sequential test assesses how much the current measurement adds to those that are less expensive.

The last k variables in a model may be tested jointly using the sequential SS output of anova for lm fits, because sequential SS are additive. Suppose that the last three variables were to be tested as a group, and that these variables had a total of 5 parameters. Then the partial F-test with 5 and n - p - 1 d.f. is the ratio of the MSR corresponding to these 3 variables to the MSE for the full model. The correct MSR is the sum of the last three sequential SS's divided by 5.

Chapter 9

The Design Library of Modeling Functions

9.1 Statistical Formulas in S

Let us first summarize many of S's general modeling capabilities. S has a battery of functions which make up a statistical modeling language [2]. At the heart of the modeling functions is an S formula of the form

$\texttt{response}\,\sim\,\texttt{terms}$

The terms represent components of a general linear model. Although variables and functions of variables make up the terms, the formula refers to additive combinations, e.g. when terms is **age** + **blood.pressure**, it refers to $\beta_1 \times age + \beta_2 \times blood.pressure$. Some examples of the terms, which describe how predictor variables are modeled, are below:

```
y \sim age + sex
                           # age + sex main effects
y \sim age + sex + age:sex \mbox{ \# add second-order interaction}
y \sim age*sex
                           # second-order interaction + all main effects
y \sim (age + sex + pressure)^2
                           # age+sex+pressure+age:sex+age:pressure...
y \sim (age + sex + pressure)^2 - sex:pressure
                           # all main effects and all 2nd order
                           # interactions except sex:pressure
y \sim (age + race)*sex
                           # age+race+sex+age:sex+race:sex
y \sim treatment*(age*race + age*sex) # no interact. with race,sex
sqrt(y) \sim sex*sqrt(age) + race
# functions, with dummy variables generated if
# race is an S factor (classification) variable
y \sim sex + poly(age,2)
                           # poly generates orthogonal polynomials
```

The formula for a regression model is given to a modeling function, e.g.

 $lrm(y \sim rcs(x,4))$

is read "use a logistic regression model to model y as a function of x, representing x by a restricted cubic spline with 4 default knots". rcs and lrm are part of Design.

You can use the S function update to re-fit a model with changes to the model terms or the data used to fit it:

The different operators that can be used to express a model are summarized in the following table As shown above, transformations of variables may be included in the formula which makes

| Expression | Meaning |
|------------|---|
| Y~M | Y is modeled as M |
| M1+M2 | Include M_1 and M_2 |
| M1-M2 | Include M_1 and leave out M_2 (-1 deletes intercept term) |
| M1:M2 | The cross-product of M_1 and M_2 |
| M1*M2 | M1+M2+M1:M2 |
| (M1+M2)^m | M_1 and M_2 and all the powers and interaction terms up to order m. |
| poly(M,n) | Orthogonal polynomial of order n |
| I() | Remove the special meaning of operators |

Table 9.1: Operators in Formulae

it very flexible. rcs in Design is the transformation for a restricted cubic spline. By default it takes 5 knots, but you can give it the number of knots or their position if you desire. lsp(age,75) fits age as a linear spline with a knot at 75 years of age (i.e., a bilinear relationship). For lsp you need to give it the position of the knots.

Transformations which involve the use of *, $\hat{}$, and | which have special meaning in this context, need to be enclosed within the function I().

9.2 Purposes and Capabilities of Design

Harrell's Design library supports biostatistical and epidemiologic modeling, testing, estimation, validation, graphics, prediction, and typesetting. The name "Design" comes from the fact that this library works by storing enhanced model design attributes in the fit. These attributes are ones needed to generate the design matrix in the first place. Design consists of about 200 functions that

9.2. PURPOSES AND CAPABILITIES OF DESIGN

assist and streamline modeling and also contains new function for binary and ordinal logistic regression models and the Buckley–James censored least squares multiple linear regression model, and implements penalized maximum likelihood estimation (shrinkage) for logistic and ordinary linear models. Design works with almost any regression model, but it was especially written to work with the models mentioned below. To use Design, you should have already installed and attached Hmisc. To access Design you need to put in the search list the directory where the functions are stored. You must force Design to be placed in front of other libraries, as Design overrides a few system–provided functions (model.frame.default and Surv being two of them):

> library(Design,T)

The Design library implements the following statistical methods.

- 1. Ordinary linear regression models
- 2. Binary and ordinal logistic models (proportional odds and continuation ratio models)
- 3. Cox model
- 4. Parametric survival models in the accelerated failure time class
- 5. Buckley–James distribution–free regression model for right–censored responses
- 6. Bootstrap model validation to obtain unbiased estimates of model performance without requiring a separate validation sample
- 7. Automatic Wald tests of all effects in the model, e.g., tests of nonlinearity of main effects when the variable does not interact with other variables, tests of nonlinearity of interaction effects, tests for whether a predictor is important, either as a main effect or as an effect modifier
- 8. Graphical depictions of model estimates (effect plots, odds/hazard ratio plots, nomograms that allow model predictions to be obtained manually even when there are nonlinear effects and interactions in the model)
- 9. Various smoothed residual plots, including some new residual plots for verifying ordinal logistic model assumptions
- 10. Composing S functions to evaluate the linear predictor $(X\hat{\beta})$, hazard function, survival function, and quantile functions analytically from the fitted model
- 11. Typesetting of fitted model using LAT_FX
- 12. Robust covariance matrix estimation (Huber or bootstrap)
- 13. Cubic regression splines with linear tail restrictions
- 14. Tensor splines (formed by taking cross-product of all spline terms of each variable)
- 15. Interactions restricted to not be doubly nonlinear
- 16. Penalized maximum likelihood estimation for ordinary linear regression and logistic regression models. Different parts of the model may be penalized by different amounts, e.g., you may want to penalize interaction or nonlinear effects more than main effects or linear effects

17. Estimation of hazard or odds ratios in presence of nonlinearity and interaction

18. Sensitivity analysis for an unmeasured binary confounder

Many of the functions in Design are organized into groups in the following tables.

| Function | Purpose | Related S Functions |
|----------|---|---------------------|
| ols | Ordinary and penalized least squares linear model | lm |
| lrm | Binary and ordinal logistic regression model | glm |
| | Has options for penalized maximum likelihood estimation | |
| psm | Accelerated failure time parametric survival models | survreg |
| cph | Cox proportional hazards regression | coxph |
| bj | Buckley–James least squares model for censored data | survreg |

 Table 9.2: Special fitting functions

The following functions have special meaning when using Design.

| Function | Purpose | Related S Functions |
|----------|--|---------------------|
| asis | No post-transformation (seldom used explicitly) | |
| rcs | Restricted cubic splines | ns |
| pol | Polynomial using standard notation | poly |
| lsp | Linear spline | |
| catg | Categorical predictor (seldom) | factor |
| scored | Ordinal categorical variables | ordered |
| matrx | Keep variables as group for anova and fastbw (seldom) | matrix |
| strat | Non-modeled stratification factors (used for cph only) | strata |

Table 9.3: Functions for transforming predictor variables in models

| Function | Purpose | Related Functions |
|-----------------|---|--------------------|
| print | Print parameters and statistics of fit | |
| coef | Fitted regression coefficients | |
| formula | Formula used in the fit | |
| specs | Detailed specifications of fit (e.g., knot locations) | |
| robcov | Robust covariance matrix estimates | |
| bootcov | Bootstrap covariance matrix estimates | |
| | and bootstrap distributions of estimates | |
| pentrace | Find optimum penalty factors by tracing | |
| | effective AIC for a grid of penalties | |
| effective.df | Print effective d.f. for each type of variable | |
| | in model, for penalized fit or pentrace result | |
| rm.impute | Impute repeated measures data with | transcan, |
| | non–random dropout | fit.mult.impute |
| summary | Summary of effects of predictors | |
| plot.summary | Plot continuously shaded confidence bars | |
| | for results of summary | |
| anova | Wald tests of most meaningful hypotheses | |
| plot.anova | Graphical depiction of anova | |
| contrast | General contrasts, C.L., tests | |
| plot | Plot effects of predictors | |
| gendata | Easily generate data with predictor combinations | |
| predict | Obtain predicted values or design matrix | |
| fastbw | Fast backward step–down variable selection | step |
| residuals | (or resid) Residuals, influence statistics from fit | |
| sensuc | Sensitivity analysis for unmeasured confounders | |
| which.influence | Which observations are overly influential | residuals |
| latex | IAT_{EX} representation of fitted model | display |
| Dialog | Create a menu to enter predictor values | Function.Design |
| | and obtain predicted values from fit | nomogram.Design |
| Function | S function analytic representation of $X\hat{\beta}$ | Function.transcan |
| | from a fitted regression model | Function.areg.boot |
| Hazard | S function analytic representation of a fitted | - |
| | hazard function (for psm) | |
| Survival | S function analytic representation of fitted | |
| | survival function (for psm,cph) | |
| Quantile | S function analytic representation of fitted | |
| | function for quantiles of survival time | |
| | (for psm, cph) | |
| Mean | S function analytic representation of fitted | |
| | function for mean survival time | |

 Table 9.4: Generic Functions and Methods

| Function | Purpose | Related S Functions |
|-----------|--|---------------------|
| nomogram | Draws a nomogram for the fitted model | latex, plot |
| survest | Estimate survival probabilities (psm, cph) | survfit |
| survplot | Plot survival curves (psm, cph) | plot.survfit |
| validate | Validate indexes of model fit using resampling | |
| calibrate | Resampling estimation of model's calibration curve | val.prob |
| vif | Variance inflation factors for fitted model | |
| naresid | Bring elements corresponding to missing data | |
| | back into predictions and residuals | |
| naprint | Print summary of missing values | |

Table 9.5: Generic Functions and Methods

The following list of topics in the online help (for Windows) for Design will also assist in understanding the components of this library.

Add to Existing Plot Bootstrap Categorical Data Character Data Operations Data Manipulation Grouping Observations **High-Level** Plots Interfaces to Other Languages Linear Algebra Logistic Regression Model Mathematical Operations Matrices and Arrays Methods and Generic Functions Nonparametric Statistics Overview **Predictive Accuracy** Printing Regression Regression and Classification Trees Robust/Resistant Techniques Sampling **Smoothing Operations** Statistical Inference Statistical Models Survival Analysis Utilities Validation of Prediction Models

See [13] for an overview of survival modeling and validation of survival models using Design. See [14] for a comprehensive case study of ordinal logistic modeling using Design. These papers also

have lots of references.

9.2.1 Differences Between lm (Builtin) and Design's ols Function

dummy variables ols uses traditional dummy variable coding.

- NA's ols deletes observations containing NA's for variables in the model. For lm you have to specify na.action=na.omit. The resid, fitted, and predict (with type='fitted') functions, when used with objects created by lm, will not hold places for NA's that were removed during the fitting process. ols holds places for NA's so that, for example, residuals can be plotted against variables in the original dataset (without having to remove observations from the variables).
- $\hat{\beta}$ The two functions compute identical coefficient and standard error estimates, assuming that ordinary dummy variable coding was used with factor variables in lm formulas.
- print print'ing an lm object results in an abbreviated summary of the model; ols prints model summary statistics (including the likelihood ratio χ^2) as well as all coefficients, standard errors, t statistics, and P-values based on the t distribution. ols also prints the adjusted R^2 and a summary of how many NA's were due to each variable in the model.
- summary summary for an lm object prints output similar to what print for an ols object prints. summary for an ols object prints estimates of effects of variables in the model (e.g., interquartile range differences in \hat{Y}).
- anova For both lm and ols F-tests are done by default and there is an option to use χ^2 tests. Unless ssType=3 is specified to anova for lm, anova prints sequential tests. anova for olsalways prints partial test statistics. So by default, anova.lm only prints partial F statistic for the final predictor in the model, and it never tests for linearity for variables that are expanded using polynomials or splines. General partial tests are obtained for lm using e.g. anova(fit.reduced,fit.full). anova for ols prints all partial tests and tests of linearity. When interactions are present, it also prints meaningful "total effect" test statistics (main effects + interaction effects combined) whereas anova for lm prints meaningless main effect tests. anova for ols also prints global (over all predictors) tests of linearity and additivity, and pooled tests involving multiple predictors can be easily specified (e.g., anova(f, sys.bp, dias.bp)).
- other functions ols fits can be used with all the other methods in Design such as nomogram, validate, and calibrate.

9.3 Examples of the Use of Design

9.3.1 Examples with Graphical Output

The first series of examples we will consider are based on binary logistic analyses of diagnostic data from the Duke Cardiovascular Disease Databank. We consider how age, sex, and serum cholesterol

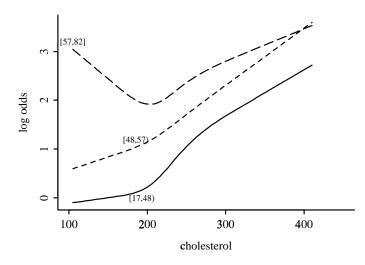


Figure 9.1: Log odds of significant coronary artery disease modeling age with two dummy variables

level relate to the probability that a patient will be found to have significant coronary artery disease by cardiac catherization (arteriography). First, to understand interactions involving age we perform an inefficient analysis in which age is stratified into tertiles. We allow for two two-way interactions but not for interaction between **sex** and **cholesterol**. We assume that the relationship between **cholesterol** and log odds of disease is smooth, by fitting a restricted cubic spline function with 4 knots. We plot the fitted model with respect to **cholesterol** and **age.tertile** by placing **cholesterol** on the x-axis and making separate curves for each age tertile. The **sex** variable is set to its reference value. In the notation **cholesterol=NA**, NA is a keyword which causes default ranges computed by **datadist** to be used. We could have given ranges explicitly, e.g.,**cholesterol=seq(100,400,by=5)**. The graph appears in Figure 9.1.

Next we obtain Wald tests of all meaningful hypotheses which can be inferred from the design:

anova(fit)

The table below was actually obtained by typing latex(anova(fit)). Next we model age more properly as a continuous variable (using a restricted cubic spline with 4 default knot locations), allowing for a general interaction surface (tensor spline) between the two continuous predictors. The surface is plotted in Figure 9.2 using default ranges, and the portion of the anova table corresponding to interactions is printed.

9.3. EXAMPLES OF THE USE OF DESIGN

| Wald Statistics | | | | | | | |
|--|----------|------|--------|--|--|--|--|
| Factor | χ^2 | d.f. | Р | | | | |
| age.tertile (Main+Interactions) | 112.62 | 10 | 0.0000 | | | | |
| All Interactions | 22.37 | 8 | 0.0043 | | | | |
| sex (Main+Interactions) | 328.90 | 3 | 0.0000 | | | | |
| All Interactions | 9.61 | 2 | 0.0082 | | | | |
| cholesterol (Main+Interactions) | 94.01 | 9 | 0.0000 | | | | |
| All Interactions | 10.03 | 6 | 0.1234 | | | | |
| Nonlinear (Main+Interactions) | 10.30 | 6 | 0.1124 | | | | |
| age.tertile * sex | 9.61 | 2 | 0.0082 | | | | |
| age.tertile * cholesterol | 10.03 | 6 | 0.1232 | | | | |
| Nonlinear Interaction : $f(A, B)$ vs. AB | 2.40 | 4 | 0.6635 | | | | |
| TOTAL NONLINEAR | 10.30 | 6 | 0.1124 | | | | |
| TOTAL INTERACTION | 22.37 | 8 | 0.0043 | | | | |
| TOTAL NONLINEAR+INTERACTION | 30.12 | 10 | 0.0008 | | | | |
| TOTAL | 404.94 | 14 | 0.0000 | | | | |

You may want to override the 3-dimensional display method used by the plot.Design function. For example, we can produce an "image" plot where for color plots the third dimension is depicted using colors of the heat spectrum and for black and white plots it is depicted using gray scale. This is done using

plot(fit, cholesterol=NA, age=NA, method='image')

| Wald Statistics | | | |
|--|----------|------|--------|
| Factor | χ^2 | d.f. | Р |
| age * cholesterol | 12.95 | 9 | 0.1649 |
| Nonlinear Interaction : $f(A, B)$ vs. AB | 7.27 | 8 | 0.5078 |
| f(A, B) vs. $Af(B) + Bg(A)$ | 5.41 | 4 | 0.2480 |
| Nonlinear Interaction in age vs. $Af(B)$ | 6.44 | 6 | 0.3753 |
| Nonlinear Interaction in cholesterol vs. $Bg(A)$ | 6.27 | 6 | 0.3931 |

The next model restricts the interaction between **age** and **cholesterol** to not be doubly nonlinear. The plot is in Figure 9.3.

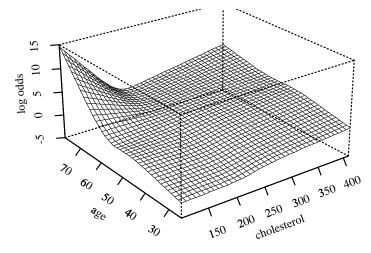


Figure 9.2: Restricted cubic spline surface in two variables, each with k = 4 knots

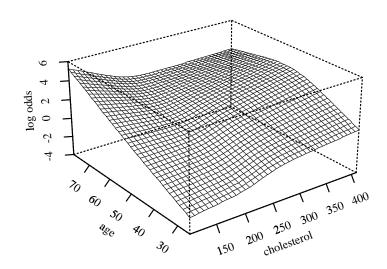


Figure 9.3: Restricted cubic spline fit with $age \times spline(cholesterol)$ and $cholesterol \times spline(age)$

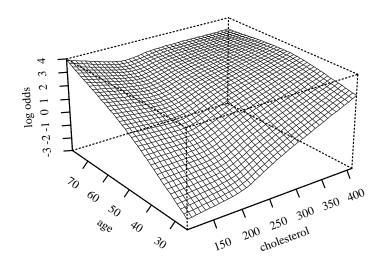


Figure 9.4: Spline fit with non-linear effects of cholesterol and age and a simple product interaction

| Wald Statistics | | | |
|--|----------|------|--------|
| Factor | χ^2 | d.f. | Р |
| age * cholesterol | 10.83 | 5 | 0.0548 |
| Nonlinear Interaction : $f(A, B)$ vs. AB | 3.12 | 4 | 0.5372 |
| Nonlinear Interaction in age vs. $Af(B)$ | 1.60 | 2 | 0.4496 |
| Nonlinear Interaction in cholesterol vs. $Bg(A)$ | 1.64 | 2 | 0.4399 |

Finally, fit a model in which the interaction between **age** and **cholesterol** is restricted to be linear in both variables (simple product form interaction). The graphical output is in Figure 9.4.

Predictions from this fit can be compared with the first model (Figure 9.1) in which age was categorized if we ask for predictions to be made at the mean age within each tertile of age. See Figure 9.5 for the result.

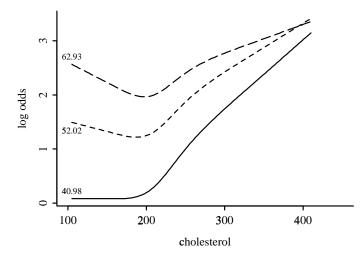


Figure 9.5: Predictions from linear interaction model with mean age in tertiles indicated

Now summarize the effects of variables from this fit. The default inter-quartile-range odds ratios are used for continuous variables. Because of the presence of interactions it is important to note the settings of interacting variables when interpreting these odds ratios. These settings are listed at the end to the output from the summary (actually summary.Design) function.

summary(fit3)

| Factor | Low | High | Diff. | Effect | S.E. | Lower | 0.95 Upper 0.95 |
|------------------------------|-----|------|-------|--------|------|-------|-----------------|
| age | 46 | 59 | 13 | 0.91 | 0.18 | 0.55 | 1.27 |
| Odds Ratio | 46 | 59 | 13 | 2.48 | NA | 1.73 | 3.55 |
| cholesterol | 196 | 259 | 63 | 0.75 | 0.14 | 0.49 | 1.02 |
| Odds Ratio | 196 | 259 | 63 | 2.13 | NA | 1.63 | 2.78 |
| <pre>sex - female:male</pre> | 1 | 2 | NA | -2.43 | 0.15 | -2.72 | -2.14 |
| Odds Ratio | 1 | 2 | NA | 0.09 | NA | 0.07 | 0.12 |

Adjusted to: age=52 sex=male cholesterol=224

This summary can also be passed to a plot method, whose results are shown in Figure 9.6. A log odds ratio scale is used.

plot(summary(fit3), log=T)

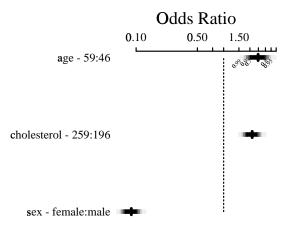


Figure 9.6: Summary of model using odds ratios and inter-quartile-range odds ratios

9.3. EXAMPLES OF THE USE OF DESIGN

Next consider a simple binary logistic model fitted to a small sample. Eighty bootstrap samples are used to compute the optimism in various indexes of model performance, and optimism is sub-tracted to obtain bias–corrected (overfitting corrected) estimates. This simple dataset is available on the UVa web page.

 $\label{eq:f} f \ \leftarrow \ \texttt{lrm}(\texttt{response} \ \sim \ \texttt{age} \ \texttt{+} \ \texttt{sex}, \ \texttt{x=T}, \ \texttt{y=T}) \\ \texttt{validate(f, B=80)}$

| Index | Original | Training | Test | Optimism | Corrected |
|-----------|----------|----------|--------|----------|-----------|
| | Sample | Sample | Sample | | Index |
| D_{xy} | 0.70 | 0.70 | 0.67 | 0.03 | 0.67 |
| R^2 | 0.34 | 0.35 | 0.32 | 0.03 | 0.31 |
| Intercept | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Slope | 0.00 | 0.00 | 0.92 | 0.08 | 0.92 |
| E_{max} | 0.00 | 0.00 | 0.02 | 0.02 | 0.02 |
| D | 0.39 | 0.41 | 0.36 | 0.05 | 0.34 |
| U | -0.05 | -0.05 | 0.01 | -0.06 | 0.01 |
| Q | 0.44 | 0.46 | 0.35 | 0.11 | 0.33 |

We can also validate a model obtained by step–down variable selection if we remember to include all candidate predictors in the fit being validated.

| Index | Original | Training | Test | Optimism | Corrected |
|-----------|----------|----------|--------|----------|-----------|
| | Sample | Sample | Sample | | Index |
| D_{xy} | 0.70 | 0.69 | 0.65 | 0.04 | 0.66 |
| R^2 | 0.34 | 0.35 | 0.31 | 0.04 | 0.30 |
| Intercept | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Slope | 1.00 | 1.00 | 0.90 | 0.10 | 0.90 |
| E_{max} | 0.00 | 0.00 | 0.02 | 0.02 | 0.02 |
| D | 0.39 | 0.41 | 0.35 | 0.06 | 0.33 |
| U | -0.05 | -0.05 | 0.01 | -0.06 | 0.01 |
| Q | 0.44 | 0.46 | 0.34 | 0.12 | 0.32 |

Factors Retained in Backwards Elimination

age sex * * * * * * * * * * * * * * * * *

Frequencies of Numbers of Factors Retained

1 2 10 70

Next turn to Cox survival modeling in a hypothetical dataset. In the following example we do not assume linearity in age, proportional hazards for sex, or additivity for age and sex. Figure 9.7 shows the model's estimates of 3-year survival probability after using the log-log transformation.

190

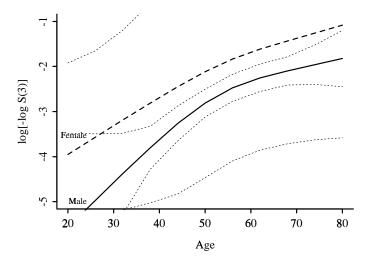


Figure 9.7: Cox PH model stratified on sex, with interaction between age spline and sex

 $\label{eq:started} \begin{array}{l} f \ \leftarrow \ cph(Srv \ \sim \ rcs(age,4) \ * \ strat(sex), \ surv=T) \\ plot(f, \ age=NA, \ sex=NA, \ time=3, \ loglog=T) \end{array}$

This model can be depicted with a nomogram. First we invoke the Survival function to compose an S function that computes survival probabilities as needed. Then we create special cases of this function to compute 3-year survival probabilities for each of the two sex strata. The two functions are needed because we are not assuming proportional hazards for sex; separate transformations of time are thus needed to compute survival probabilities. After deriving survival probability prediction functions, the Quantile function is used to compose a function to compute quantiles of survival times on demand. Then special cases are computed as before. The nomogram function is used to draw the nomogram (Figure 9.8), adding axes corresponding to the special functions just created.

| Points | <u>0</u> | 20 | | 40 | 60 | 80 | 100 |
|-----------------------------------|----------|---------------------|----------|---------------------|----------|-------------|----------------|
| age (sex=Male) age (sex=Female | | 10 10 2 0 | 20 30 | 30 40 5 0 | 40 70 | 50 60 90 | 80 |
| Total Points | 0 | 20 | • • | 40 | 60 | 80 | 100 |
| Linear Predictor | | -3 | -2 | -1 | 0 | 0.5 1 1 | .5 2 2.5 |
| S (3 Male) | | | | 0.99 | 0.98 | 0.95 0.9 | 0.8 |
| S (3 Female) | | 0.98 | 0.9 | 5 0.9 | 0.8 0 | .7 0.5 0 | .3 0 .1 |
| Median (Male) | | | | | | | 12 8 |
| Median (Female |) | | | 1 | 12 8 | 4 2 | 1 |

Figure 9.8: Nomogram from fitted Cox model

```
\begin{split} & \text{surv} \leftarrow \text{Survival(f)} \\ & \text{surv.f} \leftarrow \text{function(lp) surv(3, lp, stratum="sex=Female")} \\ & \text{surv.m} \leftarrow \text{function(lp) surv(3, lp, stratum="sex=Male")} \\ & \text{quant} \leftarrow \text{quantile(f)} \\ & \text{med.f} \leftarrow \text{function(lp) quant(.5, lp, stratum="sex=Female")} \\ & \text{at.surv} \leftarrow \text{c(.01, .05, seq(.1, .9, by=.1), .95, .98, .99, .999)} \\ & \text{at.med} \leftarrow \text{c(0, .5, 1, 1.5, seq(2, 14, by=2))} \\ & \text{nomogram(f, conf.int=F,} \\ & \text{fun=list(surv.m, surv.f, med.m, med.f),} \\ & \text{funlabel=c("S(3 | Male)", "S(3 | Female)",} \\ & & \text{"Median (Male)", "Median (Female)"),} \\ & \text{fun.at=list(at.surv, at.surv, at.med, at.med))} \end{split}
```

In the following example we assume proportional hazards for all variables and add another continuous variable to the model. This results in a nomogram (Figure 9.9) which actually requires some manual additions by the user.

| Points | 0 10 20 30 40 50 60 70 80 90 100 |
|------------------------------------|--|
| age (sex=Male) age (sex=Female) | 0 10 2 0 3 0 4 0 5 0 7 0 8 0 9 0 |
| systolic.bp | 125 135 145 155 120 105 100 95 9 0 8 5 |
| Total Points | 0 10 20 30 40 50 60 7 0 80 90 110 130 |
| Linear Predictor | -3.0 -2.0 -1.0 0.0 1.0 2.0 3.0 |
| 3y Survival Prob. | 0.99 0.95 0.80 0.60 0.30 |
| 5y Survival Prob. | 0.99 0.95 0.80 0.60 0.30 |
| Median Survival Ti | ime 14.0 4.0 1.5 |

Figure 9.9: Nomogram from fitted Cox model

Now use the latex function to typeset the fitted model. The particular latex method for cph fits also prints a table of underlying survival estimates to complete the model specification.

options(digits=3)
latex(f)

$$\operatorname{Prob}\{T \ge t \mid \operatorname{sex} = i\} = S_i(t)^{e^{X\beta}}, \text{ where }$$

$$\begin{split} X \hat{\beta} = & \\ & -3.93 \\ & +9.86 \times 10^{-2} \text{age} - 2.91 \times 10^{-5} (\text{age} - 30.7)^3_+ \\ & +8.72 \times 10^{-6} (\text{age} - 45.4)^3_+ \\ & +6.22 \times 10^{-5} (\text{age} - 54.8)^3_+ - 4.19 \times 10^{-5} (\text{age} - 69.6)^3_+ \\ & +\{\text{Female}\}[-3.50 \times 10^{-2} \text{age} + 1.90 \times 10^{-5} (\text{age} - 30.7)^3_+ \\ & -1.76 \times 10^{-5} (\text{age} - 45.4)^3_+ \\ & -2.10 \times 10^{-5} (\text{age} - 54.8)^3_+ + 1.97 \times 10^{-5} (\text{age} - 69.6)^3_+] \end{split}$$

and $\{c\} = 1$ if subject is in group c, 0 otherwise, $(x)_+ = x$ if x > 0, 0 otherwise.

| t | $S_{Male}(t)$ | $S_{Female}(t)$ |
|----|---------------|-----------------|
| 0 | 1.000 | 1.000 |
| 1 | 0.992 | 0.901 |
| 2 | 0.980 | 0.815 |
| 3 | 0.973 | 0.759 |
| 4 | 0.966 | 0.679 |
| 5 | 0.963 | 0.612 |
| 6 | 0.955 | 0.556 |
| 7 | 0.947 | 0.478 |
| 8 | 0.938 | 0.437 |
| 9 | 0.932 | 0.390 |
| 10 | 0.920 | 0.354 |
| 11 | 0.909 | 0.322 |
| 12 | 0.909 | 0.287 |
| 13 | 0.909 | 0.240 |
| 14 | 0.882 | 0.240 |

9.3.2 Binary Logistic Modeling with the Prostate Data Frame

Consider the strange task of predicting the probability of cardiovascular death (vs. alive or death due to other causes) for men with prostate cancer, allowing time until death or censoring to be a predictor variable (!).

```
> library(Design, T)  # make Design functions and datasets available
> attach(prostate)
> cvd ← status %in% c("dead - heart or vascular","dead - cerebrovascular")
> # Note: %in% is in Hmisc - makes using the match function easier
> table(cvd)
```

```
FALSE TRUE
  375 127
> f \leftarrow lrm(cvd \sim rx+rcs(dtime,5)+age+hx+bp)
> f
Logistic Regression Model
lrm(formula = cvd \sim rx + rcs(dtime, 5) + age + hx + bp)
Frequencies of Responses
FALSE TRUE
  374 127
Frequencies of Missing Values Due to Each Variable
cvd rx dtime age hx bp
  0 0
           0 1 0 0
Obs Max Deriv Model L.R. d.f. P
                                    C Dxy Gamma Tau-a R2 Brier
501
                   131.2 10 0 0.811 0.622 0.623 0.236 0.34 0.145
        2e-05
                      Coef
                              S.E. Wald Z
                                              Ρ
        Intercept -3.01327 1.41243 -2.13 0.0329
rx=0.2 mg estrogen -0.42659 0.34083 -1.25 0.2107
rx=1.0 mg estrogen -0.16740 0.34176 -0.49 0.6243
rx=5.0 mg estrogen 0.36948 0.32082 1.15 0.2495
            dtime -0.02632 0.03855 -0.68 0.4947
           dtime' 0.35472 0.25948 1.37 0.1716
          dtime'' -1.13796 0.74752 -1.52 0.1279
         dtime''' 0.78195 0.99670 0.78 0.4327
              age 0.02417 0.01829 1.32 0.1862
               hx 1.25773 0.24352 5.16 0.0000
               bp 0.17881 0.09702 1.84 0.0653
```

The fitted model object f, is a list. Let us take a look at its components.

| > names(f) | | | | | |
|------------|---------------------|----------|--------------|--|--|
| [1] | "freq" | "stats" | "fail" | | |
| [4] | "coefficients" | "var" | "u" | | |
| [7] | "deviance" | "est" | "non.slopes" | | |
| [10] | "linear.predictors" | "call" | "scale.pred" | | |
| [13] | "terms" | "assign" | "na.action" | | |
| [16] | "fail" | | | | |

Most of them are technical and needed for other functions to make calculations but a few have an immediately recognizable meaning like coefficients. One could look at them by doing something like coeff \leftarrow f\$coefficients. The preferred method however is to use functions like coeff and predict. formula can also be useful to know what model we fitted without having to print all coefficients.

cvd

There are many other arguments to lrm. Among them are the data set to be used, subset of observations to select, what to do with missing values, and whether to keep or not the design matrix and dependent variable. Look at the help files for this and other modeling functions.

Next we want to do some testing. The anova function applied to an lrm object performs a Wald test on any variable given, or all variables if no variable is given.

```
> anova(f)
```

| | Wald Statistics | | | |
|-----------|-----------------|------|--------|--|
| Factor | Chi-Square | d.f. | Р | |
| rx | 6.14 | 3 | 0.1049 | |
| dtime | 29.03 | 4 | 0.0000 | |
| Nonlinear | 25.08 | 3 | 0.0000 | |
| age | 1.75 | 1 | 0.1862 | |
| hx | 26.67 | 1 | 0.0000 | |
| bp | 3.40 | 1 | 0.0653 | |
| TOTAL | 64.07 | 10 | 0.0000 | |

If you really want to do a stepwise variable selection, the function to use is fastbw.

> fastbw(f)

P Residual d.f. Deleted Chi-Sq d.f. Ρ AIC 1.75 1 0.1862 1.75 1 0.1862 -0.25 age

Approximate Estimates after Deleting Factors

```
Coef
                              S.E. Wald Z
                                                   Ρ
         Intercept -1.22902 0.41606 -2.9539 3.138e-03
rx=0.2 mg estrogen -0.45556 0.34013 -1.3394 1.805e-01
rx=1.0 mg estrogen -0.15662 0.34167 -0.4584 6.467e-01
rx=5.0 mg estrogen 0.38155 0.32069 1.1898 2.341e-01
            dtime -0.02854 0.03852 -0.7410 4.587e-01
            dtime' 0.35037 0.25946 1.3504 1.769e-01
          dtime'' -1.11290 0.74728 -1.4893 1.364e-01
         dtime''' 0.73557 0.99608 0.7385 4.602e-01
               hx 1.29353 0.24201 5.3449 9.048e-08
               bp 0.17860 0.09702 1.8408 6.565e-02
```

Factors in Final Model

[1] rx dtime hx bp

After you run fastbw you get an estimate of the coefficients after deleting factors. The arguments to fastbw are

```
fastbw(fit, rule="aic", type="residual", sls=.05, aics=0, eps=1E-9)
```

The stopping rule can be "aic" for Akaike's information criteria or "p" for p-values. type is the type of statistic on which to base the stopping rule. type can be "residual" for pooled residual χ^2 , or "individual" for Wald χ^2 statistics of individual variables. sls and aics are cut-off values to decide when a variable is dropped from the model.

After using fastbw we may decide to refit the model dropping some variable and also on only a subset of the observations. Instead of retyping the lrm expression we can use the function update.

> f1 \leftarrow update(f,. \sim .-age,subset=dtime>20)

The arguments to update are the fitted object, the formula suitably modified, and perhaps other arguments. In the formula, we use a "." to represent the expressions that were present before and add or substract terms.

9.3.3 Troubleshooting Problems with factor Predictors

Here is an example of a problem you may encounter when using a modeling function.

```
> attach(resuse.dframe)
> m \leftarrow ols(log(billing) \sim dzgroup)
Error in lm.fit.qr(x, y, qr = ..1): computed fit is singular, rank 8
Dumped
>
> table(dzgroup)
 0:HELP only pts 1:ARF/MOSF 2:COPD 3:CHF 4:Cirrhosis 5:Coma 6:Colon Cancer
                0
                                 458
                                       726
                                                    296
                                                            247
                                                                            269
                        1513
 7:Lung Cancer 8:MOSF w/Malig
           459
                           333
```

The problem here is that the *factor* dzgroup has HELP as a possible level, but there are no patients in that category. This happens when you have a **factor** or **category** variable and there are no observations for a particular level of the variable. If importing data from SAS and there is an unused SAS PROC FORMAT VALUE label, **sas.get** will create a level for the factor anyway and since there will be no observations the resulting design matrix will be singular because one of the dummy variables is always one. The easiest way out of this problem is to run the **factor** variable through the method for subscripting factor variables as described in Section **3.4**.

```
> dzgroup ← dzgroup[] # use dzgroup[,drop=T] if Hmisc not in effect
> table(dzgroup)
1:ARF/MOSF 2:COPD 3:CHF 4:Cirrhosis 5:Coma 6:Colon Cancer 7:Lung Cancer
1513 458 726 296 247 269 459
8:MOSF w/Malig
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```

Now the new version of dzgroup will replace the old one in any subsequent calculations.

Another problem that may arise is when you want to collapse a few levels of a factor into a single level. To do this one can redefine the levels of the factor. The %in% operator can help here; see Sections 3.4 and 4.4 for other examples. Let us look at the variable group2 in the data frame.

We would like to collapse levels 6,7 and 8 into level 5. We redefine the levels attribute of group this way.

```
> levels(group) [levels(group) %in% c("6:medicine 6C","7:medicine 8B",
+ "8:medicine 9B")] \leftarrow "5:medicine"
> # '7:medicine 8B','8:medicine 9B'))
> table(group)
 1:surgery 2:cardiology 3:oncology 4:pulmonary/MICU 5:medicine
      692
                  784
                            757
                                            886
                                                     1172
9:medical house staff 10:surgical house staff
                   0
                                         0
> # Now delete unused levels
                   $ group[,drop=T] if Hmisc not in effect
> group \leftarrow group[]
> table(group)
   1:surgery 2:cardiology 3:oncology 4:pulmonary/MICU 5:medicine
 10
         692
                     784
                               757
                                               886
                                                        1172
```

Notice that the values of medicine 6C, 8B, 9B etc have been correctly collapsed into medicine.

9.3.4 A Comprehensive Hypothetical Example

As another example of using many of the Design functions (as well as the describe and impute functions in Hmisc), suppose that a categorical variable treat has values "a", "b", and "c", an ordinal variable num.diseases has values 0,1,2,3,4, and that there are two continuous variables, age and cholesterol. age is fitted with a restricted cubic spline, while cholesterol is transformed using the transformation log(cholesterol+10). Cholesterol is missing on three subjects, and we impute these using the overall median cholesterol. We wish to allow for interaction between treat and cholesterol. The following S program will fit a logistic model, test all effects in the design, estimate effects, and plot estimated transformations. The fit for num.diseases really considers the variable to be a 5-level categorical variable. The only difference is that a 3 d.f. test of linearity is done to assess whether the variable can be re-modeled "asis". Here we also show statements to store predictor characteristics from datadist.

```
library(Design, T)
options(datadist="ddist")
                            # defines data dist. to Design
cholesterol ← impute(cholesterol)
fit \leftarrow lrm(y \sim treat + scored(num.diseases) + rcs(age) +
              log(cholesterol+10) + treat:log(cholesterol+10))
describe(y \sim treat + scored(num.diseases) + rcs(age))
# or use describe(formula(fit)) for all variables used in fit
# describe function (in Hmisc) gets simple statistics on variables
#fit ← robcov(fit)
                            # Would make all statistics which follow
                            # use a robust covariance matrix
                            # would need x=T, y=T in lrm()
specs(fit)
                            # Describe the design characteristics
anova(fit)
```

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```
anova(fit, treat, cholesterol)  # Test these 2 by themselves
plot(anova(fit))
                              # Summarize anova graphically
summary(fit)
                              # Estimate effects using default ranges
plot(summary(fit))
                              # Graphical display of effects with C.L.
summary(fit, treat="b", age=60) # Specify reference cell and adjustment val
summary(fit, age=c(50,70))
                              # Estimate effect of increasing age from
                              # 50 to 70
summary(fit, age=c(50,60,70))
                              # Increase age from 50 to 70, adjust to
                              # 60 when estimating effects of other factors
# If had not defined datadist, would have to define ranges for all var.
plot(fit, age=seq(20,80,length=100), treat=NA, conf.int=F)
                              # Plot relationship between age and log
                              # odds, separate curve for each treat,
                              # no C.I.
plot(fit, age=NA, cholesterol=NA)# 3-dimensional perspective plot for age,
                              # cholesterol, and log odds using default
                              # ranges for both variables
plot(fit, num.diseases=NA, fun=function(x) 1/(1+exp(-x)) ,
    ylab="Prob", conf.int=.9) # Plot estimated probabilities instead of
                              # log odds
# Again, if no datadist were defined, would have to tell plot all limits
# Estimate and test treatment (b-a) effect averaged over 3 cholesterols
contrast(fit, list(treat='b', cholesterol=c(150,200,250)),
             list(treat='a', cholesterol=c(150,200,250)),
        type='average')
cholesterol=seq(100,300,length=10)))
# Could also obtain list of predictor settings interactively
# Since age doesn't interact with anything, we can quickly and
# interactively try various transformations of age, taking the spline
# function of age as the gold standard. We are seeking a linearizing
# transformation.
ag \leftarrow 10:80
cholesterol=median(cholesterol)),
               type="terms")[,"age"]
# Note: if age interacted with anything, this would be the age
       "main effect" ignoring interaction terms
# Could also use
    logit \leftarrow plot(f, age=ag, ...)$x.xbeta[,2]
#
# which allows evaluation of the shape for any level of interacting
# factors. When age does not interact with anything, the result from
# predict(f, ..., type="terms") would equal the result from
# plot if all other terms were ignored
```

The following is a typical sequence of steps that would be used with Design in conjunction with the Hmisc transcan function to do single imputation of all NAs in the predictors¹, fit a model, do backward stepdown to reduce the number of predictors in the model (with all the severe problems this can entail), and use the bootstrap to validate this stepwise model, repeating the variable selection for each re-sample. Here we take a short cut as the imputation is not repeated within the bootstrap. In what follows we (atypically) have only 3 candidate predictors. In practice be sure to have the validate and calibrate functions operate on a model fit that contains all predictors that were involved in previous analyses that used the response variable. Here the imputation is necessary because backward stepdown would otherwise delete observations missing on any candidate variable.

```
xt <- transcan(~ x1 + x2 + x3, imputed=T)
impute(xt) # imputes any NAs in x1, x2, x3
# Now fit original full model on filled-in data
f <- lrm(y ~ x1 + rcs(x2,4) + x3, x=T, y=T) # x,y allow boot.
fastbw(f) # derive stepdown model (using default stopping rule)
validate(f, B=100, bw=T) # repeats fastbw 100 times
cal <- calibrate(f, B=100, bw=T) # also repeats fastbw
plot(cal)
```

See Section 13.2 for a much more comprehensive example of the use of Design.

9.3.5 Using Design and Interactive Graphics to Generate Flexible Functions

Sometimes one wishes to simulate data from a complex non-monotonic regression relationships. In this example we open an empty plot, draw a curve using mouse clicks, fit the function using least squares via a spline function, and create an S function representing a close approximation to the manually drawn function. This latter function can then be used inside a simulation loop to create a population predictor effect, for example. This example also shows how restricted cubic splines are fitted. You may have to specify knot locations yourself to fit the tails of the curve adequately if you don't click the mouse very rapidly there.

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 $^{^{1}}$ Multiple imputation would be better but would be harder to do in the context of bootstrap model validation.

```
plot(0,0, xlim=c(0,1), ylim=c(0,1)) # open empty graph
z \leftarrow locator(type='b')
                                        # return points until right mouse button
                                        # clicked, drawing pts and lines
x1 \leftarrow z$x
                                        # pull off x-coordinates
                                        # pull off y-coordinates
y ← z$y
w \leftarrow datadist(x1)
options(datadist='w')
h \leftarrow ols(y ~ rcs(x1,6))
                                        # least squares fit
plot(h, add=T, conf.int=F, col=2)
                                        # show fitted curve
                                        # represent fit as an S function
hf \leftarrow Function(h)
xx \leftarrow seq(0,1,length=100)
                                        # grid of points to evaluate
lines(xx, hf(xx), lwd=2, col=2)
                                        # re-draw fitted curve
```

9.4 Checklist of Problems to Avoid When Using Design

- 1. Don't have a formula like y ~ age + age^2. In S you need to connect related variables using a function which produces a matrix, such as pol or rcs. This allows effect estimates (e.g., hazard ratios) to be computed as well as multiple d.f. tests of association.
- 2. Don't use poly or strata inside formulas used in Design. Use pol and strat instead.
- 3. Almost never code your own dummy variables or interaction variables in S. Let S do this automatically. Otherwise, **anova** and other functions can't do their job.
- 4. Almost never transform predictors outside of the model formula, as then plots of predicted values vs. predictor values, and other displays, would not be made on the original scale. Use instead something like y ~ log(cell.count+1), which will allow cell.count to appear on x-axes. You can get fancier, e.g., y ~ rcs(log(cell.count+1),4) to fit a restricted cubic spline with 4 knots in log(cell.count+1). For more complex transformations do something like

```
f ← function(x) {
    ... various 'if' statements, etc.
    log(pmin(x,50000)+1)
}
fit1 ← lrm(death ~ f(cell.count))
fit2 ← lrm(death ~ rcs(f(cell.count),4))
```

- 5. Don't put \$ inside variable names used in formulas. Either attach data frames or use data=.
- 6. Don't forget to use datadist and options(datadist=...). Try to use it at the top of your program so that all model fits can automatically take advantage if its distributional summaries for the predictors.
- 7. Don't validate or calibrate models which were reduced by dropping "insignificant" predictors. Proper bootstrap or cross-validation must repeat any variable selection steps for each re-sample. Therefore, validate or calibrate models which contain all candidate predictors, and if you must reduce models, specify the option bw=T along with any non-default stopping rules when you run validate or calibrate.

- 8. Dropping of "insignificant" predictors ruins much of the usual statistical inference for regression models (confidence limits, standard errors, P-values, χ^2 , ordinary indexes of model performance) and it also results in models which will have worse predictive discrimination.
- 9. Make sure you include the T in library(Design, T), and do library(Design, T) after library(Hmisc, T)

9.5 Describing Representation of Subjects

The Hmisc dataRep function is useful for describing how well a new subject was represented in a dataset used to develop a predictive model. This can supplement confidence intervals in guarding against over-interpretation when extrapolation is done.

Chapter 10

Principles of Graph Construction

The ability to construct clear and informative graphs is related to the ability to understand the data. There are many excellent texts on statistical graphics (many of which are listed at the end of this chapter). Some of the best are Cleveland's 1994 book *The Elements of Graphing Data* and the books by Tufte. The suggestions for making good statistical graphics outlined here are heavily influenced by Cleveland's books, and quotes below are from his 1994 book.

10.1 Graphical Perception

- Goals in communicating information: reader perception of data values and of data patterns. Both accuracy and speed are important.
- Pattern perception is done by

detection : recognition of geometry encoding physical values

assembly : grouping of detected symbol elements

estimation : assessment of relative magnitudes of two physical values

- For estimation, many graphics involve discrimination, ranking, and estimation of ratios
- Humans are not good at estimating differences without directly seeing differences (especially for steep curves)
- Humans do not naturally order color hues
- Only a limited number of hues can be discriminated in one graphic
- Weber's law: The probability of a human detecting a difference in two lines is related to the ratio of the two line lengths

- This is why grid lines and frames improve perception and is related to the benefits of having multiple graphs on a common scale.
 - eye can see ratios of filled or of unfilled areas, whichever is most extreme
- For categorical displays, sorting categories by order of values attached to categories can improve accuracy of perception. Watch out for over-interpretation of extremes though.
- The aspect ratio (height/width) does not have to be unity. Using an aspect ratio such that the average absolute curve angle is 45° results in better perception of shapes and differences (banking to 45°).
- Optical illusions can be caused by:
 - hues, e.g., red is emotional. A red area may be perceived as larger.
 - shading; larger regions appear to be darker
 - orientation of pie chart with respect to the horizon
- Humans are bad at perceiving relative angles (the principal perception task used in a pie chart)
- Here is a hierarchy of human graphical perception abilities:
 - 1. Position along a common scale (most accurate task)
 - 2. Position along identical nonaligned scales
 - 3. Length
 - 4. Angle and slope
 - 5. Area
 - 6. Volume
 - 7. Color: hue (red, green, blue, etc.), saturation (pale/deep), and lightness
 Hue can give good discrimination but poor ordering

10.2 General Suggestions

- Exclude unneeded dimensions (e.g. width, depth of bars)
- "Make the data stand out. Avoid Superfluity"; Decrease ink to information ratio
- "There are some who argue that a graph is a success only if the important information in the data can be seen in a few seconds. ... Many useful graphs require careful, detailed study."
- When actual data points need to be shown and they are too numerous, consider showing a random sample of the data.
- Omit "chartjunk"
- Keep continuous variables continuous; avoid grouping them into intervals. Grouping may be necessary for some tables but not for graphs.
- Beware of subsetting the data finer than the sample size can support; conditioning on many variables simultaneously (instead of multivariable modeling) can result in very imprecise estimates

10.3 Tufte on "Chartjunk"

Chartjunk does not achieve the goals of its propagators. The overwhelming fact of data graphics is that they stand or fall on their content, gracefully displayed. Graphics do not become attractive and interesting through the addition of ornamental hatching and false perspective to a few bars. Chartjunk can turn bores into disasters, but it can never rescue a thin data set. The best designs ... are *intriguing and curiosity-provoking*, drawing the viewer into the wonder of the data, sometimes by narrative power, sometimes by immense detail, and sometimes by elegant presentation of simple but interesting data. But no information, no sense of discovery, no wonder, no substance is generated by chartjunk.

Tufte p. 121, 1983

10.4 Tufte's Views on Graphical Excellence

"Excellence in statistical graphics consists of complex ideas communicated with clarity, precision, and efficiency. Graphical displays should

- show the data
- induce the viewer to think about the substance rather than about methodology, graphic design, the technology of graphic production, or something else
- avoid distorting what the data have to say
- present many numbers in a small space
- make large data sets coherent
- encourage the eye to compare different pieces of data
- reveal the data at several levels of detail, from a broad overview to the fine structure
- serve a reasonably clear purpose: description, exploration, tabulation, or decoration
- be closely integrated with the statistical and verbal descriptions of a data set."

10.5 Formatting

- Tick Marks should point outward
- x- and y-axes should intersect to the left of the lowest x value and below the lowest y value, to keep values from being hidden by axes
- Minimize the use of remote legends. Curves can be labeled at points of maximum separation (see the Hmisc labcurve function).

10.6 Color, Symbols, and Line Styles

- Some symbols (especially letters and solids) can be hard to discern
- Use hues if needed to add another dimension of information, but try not to exceed 3 different hues. Instead, use different saturations in each of the three different hues.
- Make notations and symbols in the plots as consistent as possible with other parts, like tables and texts
- Different dashing patterns are hard to read especially when curves inter-twine or when step functions are being displayed
- An effective coding scheme for two lines is to use a thin black line and a thick gray scale line

10.7 Scaling

- Consider the inclusion of 0 in your axis. Many times it is essential to include 0 to tell the full story. Often the inclusion of zero is unnecessary.
- Use a log scale when it is important to understand percent change of multiplicative factors or to cure skewness toward large values
- Humans have difficulty judging steep slopes; bank to 45°, i.e., choose the aspect ratio so that average absolute angle in curves is 45°.

10.8 Displaying Estimates Stratified by Categories

- Perception of relative lengths is most accurate areas of pie slices are difficult to discern
- Bar charts have many problems:
 - High ink to information ratio
 - Error bars cause perception errors
 - Can only show one-sided confidence intervals well
 - Thick bars reduce the number of categories that can be shown
 - Labels on vertical bar charts are difficult to read
- Dot plots are almost always better
- Consider multi-panel side-by-side displays for comparing several contrasting or similar cases. Make sure the scales in both x and y axes are the same across different panels.
- Consider ordering categories by values represented, for more accurate perception

10.9 Displaying Distribution Characteristics

- When only summary or representative values are shown, try to show their confidence bounds or distributional properties, e.g., error bars for confidence bounds or box plot
- It is better to show confidence limits than to show ± 1 standard error
- Often it is better still to show variability of *raw* values (quartiles as in a box plot so as to not assume normality, or S.D.)
- For a quick comparison of distributions of a continuous variable against many categories, try box plots.
- When comparing two or three groups, overlaid empirical distribution function plots may be best, as these show all aspects of the distribution of a continuous variable.

10.10 Showing Differences

- Often the only way to perceive differences accurately is to actually compute differences; then plot them
- It is not a waste of space to show stratified estimates and differences between them on the same page using multiple panels
- This also addresses the problem that confidence limits for differences cannot be easily derived from intervals for individual estimates; differences can easily be significant even when individual confidence intervals overlap.
- Humans can't judge differences between steep curves; one needs to actually compute differences and plot them.

The plot in figure 10.1 shows confidence limits for individual means, using the nonparametric bootstrap percentile method, along with bootstrap confidence intervals for the difference in the two means. The code used to produce this figure is below.

```
\begin{array}{l} \mbox{attach}(\mbox{diabetes}) \\ \mbox{bootmean} \leftarrow \mbox{function}(x, B=1000) \{ \\ w \leftarrow \mbox{smean.cl.boot}(x, B=B, \mbox{reps}=T) \\ \mbox{reps} \leftarrow \mbox{attr}(w, \mbox{reps}') \\ \mbox{attr}(w, \mbox{reps}') \leftarrow \mbox{NULL} \\ \mbox{list}(\mbox{stats}=w, \mbox{reps}=\mbox{reps}) \\ \mbox{set.seed}(1) \\ \mbox{male} \leftarrow \mbox{bootmean}(\mbox{glyhb}[\mbox{gender}=='\mbox{male}']) \\ \mbox{dif} \leftarrow \mbox{comman}(\mbox{glyhb}[\mbox{gender}=='\mbox{male}']) \\ \mbox{dif} \leftarrow \mbox{comman}(\mbox{glyhb}[\mbox{gender}=='\mbox{female}']) \\ \mbox{dif} \leftarrow \mbox{comman}(\mbox{glyhb}[\mbox{gender}=='\mbox{female}']) \\ \mbox{male} \leftarrow \mbox{bootmean}(\mbox{glyhb}[\mbox{gender}=='\mbox{female}']) \\ \mbox{male} \leftarrow \mbox{mean}=\mbox{ads}\mbox{stats}['\mbox{Mean}'] - \mbox{female}\mbox{stats}['\mbox{Mean}'], \\ \mbox{quantile}(\mbox{male}\mbox{stats} ['\mbox{Mean}'] - \mbox{female}\mbox{stats}['\mbox{Mean}'], \\ \mbox{male} \leftarrow \mbox{male}\mbox{stats} \\ \mbox{par}(\mbox{mar}=\mbox{c}(4,6,4,1)) \\ \mbox{plot}(0,0,\mbox{stats}'\mbox{Glycated}\mbox{Hemoglobin}',\mbox{ylab}='', \\ \mbox{xlim}=\mbox{c}(5,6.5),\mbox{ylim}=\mbox{c}(0,4),\mbox{axes}=\mbox{F}) \\ \mbox{axis}(1) \end{array}
```

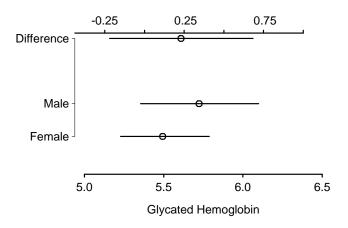


Figure 10.1: Means and nonparametric bootstrap 0.95 confidence limits for glycated hemoglobin for males and females, and confidence limits for males - females. Lower and upper x-axis scales have same spacings but different centers. Confidence intervals for differences are generally wider than those for the individual constituent variables.

```
axis(2, at=c(1,2,4),
    labels=c('Female', 'Male', 'Difference'),
    las=1, adj=1, lwd=0)
points(c(male[1], female[1]), 2:1)
segments(female[2], 1, female[3], 1)
segments(male[2], 2, male[3], 2)
offset ← mean(c(male[1], female[1])) - dif[1]
points(dif[1] + offset, 4)
segments(dif[2]+offset, 4, dif[3]+offset, 4)
at ← c(-.5, -.25, 0, .25, .5, .75, 1)
axis(3, at=at+offset, label=format(at))
```

10.11 Choosing the Best Graph Type

The recommendations that follow are good on the average, but be sure to think about alternatives for your particular data set. For nonparametric trend lines, it is advisable to add a "rug" plot to show the density of the data used to make the nonparametric regression estimate. Alternatively, use the bootstrap to derive nonparametric confidence bands for the nonparametric smoother.

10.11.1 Single Categorical Variable

Use a dot plot or horizontal bar chart to show the proportion corresponding to each category. Second choices for values are percentages and frequencies. The total sample size and number of missing

10.12. CONDITIONING VARIABLES

values should be displayed somewhere on the page. If there are many categories and they are not naturally ordered, you may want to order them by the relative frequency to help the reader estimate values.

10.11.2 Single Continuous Numeric Variable

An empirical cumulative distribution function, optionally showing selected quantiles, conveys the most information and requires no grouping of the variable. A box plot will show selected quantiles effectively, and box plots are especially useful when stratifying by multiple categories of another variable. Histograms are also possible.

10.11.3 Categorical Response Variable vs. Categorical Ind. Var.

This is essentially a frequency table. It can also be depicted graphically (Section 6.3).

10.11.4 Categorical Response vs. a Continuous Ind. Var.

Choose one or more categories and use a nonparametric smoother to relate the independent variable to the proportion of subjects in the categories of interest. Show a rug plot on the x-axis.

10.11.5 Continuous Response Variable vs. Categorical Ind. Var.

If there are only two or three categories, superimposed empirical cumulative distribution plots with selected quantiles can be quite effective. Also consider box plots, or a dot plot with error bars, to depict the median and outer quartiles. Occasionally, a back-to-back histogram can be effective for two groups (see the Hmisc histbackback function).

10.11.6 Continuous Response vs. Continuous Ind. Var.

A nonparametric smoother is often ideal. You can add rug plots for the x- and y-axes, and if the sample size is not too large, plot the raw data. If you don't trust nonparametric smoothers, group the x-variable into intervals having a given number of observations, and for each x-interval plot characteristics (3 quartiles or mean ± 2 SD, for example) vs. the mean x in the interval. This is done automatically with the Hmisc xYplot function with the methods='quantile' option.

10.12 Conditioning Variables

You can condition (stratify) on one or more variables by making separate pages by strata, by making separate panels within a page, and by superposing groups of points (using different symbols or colors) or curves within a panel. The actual method of stratifying on the conditional variable(s) depends on the type of variables.

Categorical variable(s) : The only choice to make in conditioning (stratifying) on categorical variables is whether to combine any low-frequency categories. If you decide to combine them on the basis of relative frequencies you can use the combine.levels function in Hmisc.

Continuous numeric variable(s) : Unfortunately, to condition on a continuous variable without the use of a parametric statistical model, one must split the variable into intervals. The first choice is whether the intervals of the numeric variable should be overlapping or non-overlapping. For the former the built-in equal.count function can be used for a paneling or grouping variable in trellis graphics (these overlapping intervals are called "shingles" in trellis). For non-overlapping intervals the Hmisc cut2 function is a good choice because of its many options and compact labeling.

biostat.mc.vanderbilt.edu/StatGraphCourse has more information on statistical graphics
and links to pertinent sites.

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Chapter 11

Graphics in S

11.1 Overview

S has a large variety of plotting routines. In order to be able to display a plot one needs to open a special window for this purpose as described in Section 12.2. For example, UNIX users might open a graphics window using X11() or motif(), and Windows 3.3 users usually use win.graph(), while 4.x or later Windows users let the system open a graph sheet.

We will begin this chapter by covering some of the lower-level plotting functions, then we will move up to the higher-level multi-way trellis graphics (which generalize the coplot function). All of the basic graphs and many trellis-type graphs can be produced in S-PLUS 4.x or later using dialog boxes, and graphs can be edited and annotated interactively using point-and-click. All this is usually done by clicking on a data frame in the left pane of the Object Browser to get a list of the frame's variables in the right pane. Then one or more variable names are highlighted (using left click or control-left-click) and a graph type is clicked on a 2D or 3D graphics palette. However, with our slant of being able to reproduce analyses when data are updated, we will present only the command interface in this chapter.

In 4.x or later you can edit an S-PLUS graph, whether it was produced by a dialog or by commands, using the S-PLUS graphics editor, or you can even edit the graph in Microsoft Word or Powerpoint when the editing process requires S-PLUS to manipulate graphics objects. This is done through dynamic object linking in Windows 95. Also take a look at Metafile Companion for editing Windows metafiles, as described briefly in Section 1.9.

The typical plotting command is of the form plot(fun1(var1),fun2(var2),...). This will plot a transformation (fun2) of var2 on the y-axis vs. the transformation fun1 of var1 on the x-axis. The ... represent graphical parameters to pass to plot to control different aspects of the plot such as plot size, labeling of axes, position of the plot on the paper, orientation, limits for the axes, line type, number of plots to a page, etc.

Graphical parameters can be passed to plot as part of its arguments, or be defined beforehand through the par(...) function. In this latter case, they remain in effect for the duration of the

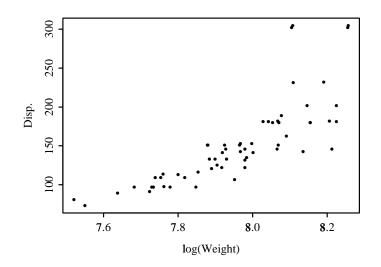


Figure 11.1: Basic Plot

S session, while in the former they are only active for that particular **plot** command. There are many graphical parameters and we can classify them in basically four groups: parameters affecting graphical elements (lines, points, polygons and so on), parameters affecting axes and tick marks, parameters affecting margins and parameters affecting a multiple figure layout. Let's do some examples using the car.test.frame dataframe that is supplied with S-PLUS.

```
> attach(car.test.frame)
> names(car.test.frame)
[1] "Price" "Country" "Reliability" "Mileage" "Type"
[6] "Weight" "Disp." "HP"
> plot(log(Weight),Disp.)
```

The results are shown in Figure 11.1.

Axes are labeled with variable names and they are scaled to include all observations in the data frame. We will improve it a little bit by adding titles, a smooth fitting line and axis labels

```
> plot(log(Weight),Disp.,xlab="Log of Weight",
+ ylab="Displacement",
+ main="Displacement vs log of Weight")
> lines(supsmu(log(Weight),Disp.))
```

If at this point we wanted to print the plot, there is an option in the graphics window to do so (in UNIX, click the right mouse button on **Graph** and choose **Print** from the menu). You can also make a copy of the plot in a smaller window or resize it to your preferences). For Windows 4.x and later you use the **Print Graph Sheet Page** command in the **File** menu. In the example above, the arguments for labels and titles could have been given in a different command title(main,sub,xlab,ylab). The command lines(x,y) adds lines with coordinates determined by the vectors x and y (it could also be a matrix with two columns). Here, the role of x and y is played by the pair of vectors returned

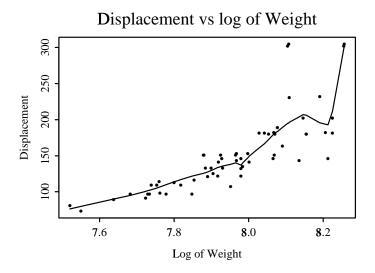


Figure 11.2: Basic Plot with Labels and Title

by supsmu which determine a non-parametric smooth fit. lowess is another function which does smooth fitting note that you must remove NAs yourself to use it. A function similar in purpose to lines is points. The results are shown in Figure 11.2.

Let us look at the distribution of mileage by type of car. Let us try

> plot(Type,Mileage,boxmeans=T,rotate=T)

Here, again we see how S is smart enough to recognize that Type is a factor variable and does a boxplot. The arguments **boxmeans** and **rotate** display the mean **Mileage** by Type and rotate labels on the *x*-axis. However, to do boxplots, the **boxplot** function is preferred due to its greater flexibility.

> boxplot(split(Mileage,Type),varwidth=T,notch=T)

The split function here is needed to classify Mileage by Type. The argument varwidth specifies that the box widths is proportional to the square root of the number of observation in each box. The notch arguments provide notches that can be used for a rough significance test at the 5% level.

Let us examine how plot behaves on fitted models. (plot acts differently on models not fitted with a Design function).

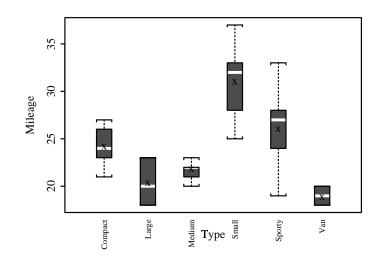


Figure 11.3: Plotting a Factor

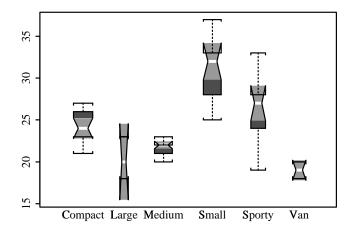


Figure 11.4: Example of Boxplot

```
> f \leftarrow ols(Mileage \sim Weight+Type+Disp.,x=T)
> f
Least Squares Regression Model
ols(formula = Mileage \sim Weight + Type + Disp.)
n=60
      p=7
Residuals:
   Min
           10 Median 30
                             Max
-5.515 -1.141 -0.05707 1.54 4.715
Coefficients:
              Value Std. Error t value Pr(>|t|)
 Intercept 33.9640 4.1053
                                8.2733
                                        0.0000
    Weight -0.0017 0.0018
                               -0.9152
                                         0.3643
Type=Large
            2.6627 1.8435
                                1.4444
                                        0.1546
Type=Medium -0.4514 0.9673
                               -0.4666
                                         0.6427
Type=Small
            4.3597 1.1194
                                3.8948
                                        0.0003
Type=Sporty
            2.6860 0.9985
                                2.6900
                                        0.0096
  Type=Van -3.2339 1.4875
                               -2.1740
                                         0.0343
     Disp. -0.0361 0.0124
                               -2.9100
                                         0.0053
Residual standard error: 2.238 on 52 degrees of freedom
```

```
Multiple R-Squared: 0.8077 Adjusted R-Squared: 0.7818
```

plot can be applied to fitted models to display how the response function behaves as the predictors in the model vary. When using plot with Design for this purpose we need to tell the function how to adjust the predictors that are not being plotted. This can be done in two ways: by passing them explicitly to plot as arguments, or by means of the datadist function. datadist takes a dataframe or a list of variable names and returns an object of class "datadist" with information that helps plot determine the limits of the variables being plotted, and adjustments for other variables in the model. We then set the options(datadist=...) parameter which instructs S where to point to find the limits for the variables. For example

Values:

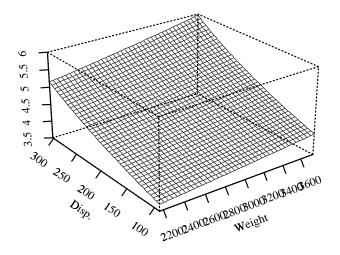


Figure 11.5: Example of Plot on a Fitted Model

Type : Compact Large Medium Small Sporty Van

This is saying that if we want to plot the predicted values from f as a function of Weight and Disp., they will range from 2165.25 to 3735.00 and 90.90 to 302.00 respectively, while the Type factor will be adjusted to the value Compact. To specify that we want plot to cover the full range determined by datadist we use NA by convention

```
> plot(f,Weight=NA,Disp.=NA,fun=function(x) 100/x)
```

In this example we chose to represent a transformation of the response (100/x) by defining it in line through the fun= argument. This is a feature common to many S functions. If we wanted to use a factor rather than a continuous variable as a predictor we would have obtained one curve for each level of the factor plus confidence intervals.

We can override the values chosen by datadist as limits and adjustment

> plot(f,Disp.=seq(150,250,by=5),Type=NA,Weight=2800,conf.int=F)

How does plot manage to behave so differently depending on the kind of arguments we give it? The answer is in the class attribute of its main argument. If we try to look at the plot function itself we get

```
> plot
function(x, ...)
UseMethod("plot")
```

What this means is that when we type plot(x), plot looks at the class attribute of x, say z, and then calls the function plot.z which will produce the appropriate plot.

```
> class(f)
```

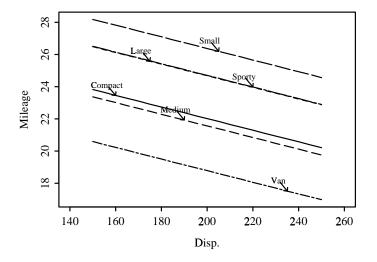


Figure 11.6: Overriding datadist Values

```
"Design" "lm"
[1] "ols"
> args(plot.ols)
Error: Object "plot.ols" not found
Dumped
> args(plot.Design)
function(fit, ..., xlim, ylim, fun, xlab, ylab, conf.int = 0.95, add = F,
        label.curves = T, eye, lty, col = 1, adj.zero = F, ref.zero = F,
        adj.subtitle, cex.adj = 1, non.slopes, time, loglog = F, val.lev = F,
        digits = 4, cex.label = 0.75)
> class(site)
[1] "factor"
> args(plot.factor)
function(x, y = NULL, ..., style = "box", rotate = sum(nchar(xalabs)) > 80,
       boxmeans = F, character, xlab = fn, ylab = yname, ylim = ymm, ask = T,
       data = NULL)
```

This is showing that an object can have more than one class attribute and plot will look at all of them starting from the left until it finds a function of the form plot.z. This behavior is not restricted to plot. Many other functions such as print, summary and anova also act this way. They are called *generic* functions and *methods* can be written for them, meaning special functions to handle special objects. One consequence of this software design is that when we look up help, we want to make sure that we are looking for help for the correct function. For example help(anova) will give us help for the S anova function, while help(anova.Design) will give us help on Design's anova function.

Two other plotting functions that we want to look at are qqnorm and coplot. qqnorm (complemented by qqline) does a normal probability plot. In our example we may want to check if the residuals from the fitted model are normally distributed. We could extract the residuals by using resid and then type

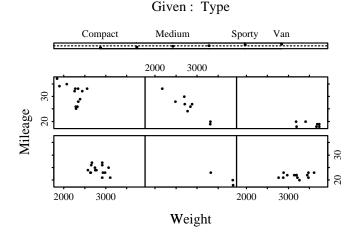


Figure 11.7: Example of Co-Plot

```
> qqnorm(resid(f))
> qqline(resid(f))
```

There are functions to do quantile-quantile plots for other distributions (See [7,section 5.5.4.1)).

If we want to see how Mileage depends on Weight across the different types we can do a *conditioning plot* or *coplot*.

coplot(y \sim x|z, given.values=z, panel=panel.smooth)

gives a scatterplot of y vs x conditioning on the values of z. z could be a factor or a series of overlapping (or not) intervals. In this latter case, if z is divided into, say, m intervals, then m plots of y vs x are done with the variables restricted to those intervals. When z is a factor we get one plot for each level of the the factor.

```
> coplot(Mileage \sim Weight|Type)
```

The labeling here is a little unusual since it starts from left to right and from bottom to top. The idea is that it should be read like any other graph, with the origin in the bottom left of the page and values on the x-axis increasing to the right, and values on the y-axis increasing upwards. The key on how to read it is given by the top panel. If z is a continuous variable the function co.intervals could be used to construct the intervals. It doesn't matter what function we use to construct them as long as the end result is a matrix with two columns and the interval extremes as rows.

There are many other plotting functions. Two that are worth exploring are pairs and interaction.plot.

11.2 Adding Text or Legends and Identifying Observations

In the example above, we fitted a least squares model to Mileage. We specified x=T to store the design matrix along with the fit. Using this information we can now use the function which.influence to

extract influential observations

```
> w ← which.influence(f,cutoff=.5)
> w
$Intercept:
[1] "Ford Festiva 4" "Honda Civic CRX Si 4"
$Weight:
[1] "Ford Festiva 4"
$Type:
[1] "Ford Festiva 4"
```

w is a list with one component for each factor with influential observations according to a criteria defined by the cutoff= argument. Each component lists the observations that unduly affect that particular coefficient. We would like to refit the model dropping this observations. This is a good time to use unlist.

unlist makes the list w into a vector but one with repeated components and not sorted. This is solved by using unique and sort. Then we use match to get a vector with the indexes of car.test.frame corresponding to the influential observations. We can use them to extract those elements not in wu.

```
> fu <- update(f,. ~ .,subset=row.names(car.test.frame)[-wuc],x=F)
> fu
Least Squares Regression Model
ols(formula = Mileage \sim Weight + Disp. + Type, subset = row.names(
       car.test.frame)[ - wuc], x = F)
n=58
     p=7
Residuals:
   Min
          1Q Median
                     3Q Max
 -5.067 -1.216 0.103 1.188 4.245
Coefficients:
             Value Std. Error t value Pr(>|t|)
 Intercept 28.0726 4.1988 6.6859 0.0000
    Weight 0.0007 0.0018
                               0.3771 0.7077
     Disp. -0.0421 0.0117
                              -3.6100 0.0007
 Type=Large 1.4479 1.7522
                              0.8263 0.4125
```

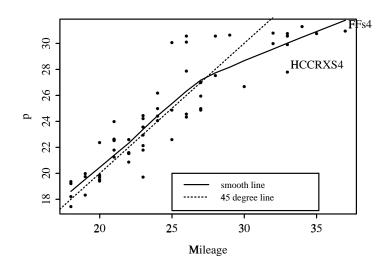


Figure 11.8: Identifying Observations

| Type=Medium Type=Small | | 0.9186 1.0654 | -1.2347 4.6739 | 0.2227 0.0000 | | |
|--|---------|------------------|-------------------|------------------|--|--|
| Type=Sporty | 2.3026 | 0.9553 | 2.4104 | 0.0197 | | |
| Type=Van | -4.7508 | 1.4495 | -3.2775 | 0.0019 | | |
| Residual standard error: 2.067 on 50 degrees of freedom Multiple R-Squared: 0.8096 Adjusted R-Squared: 0.7829 | | | | | | |
| $ angle 	ext{p} \leftarrow 	ext{predict(fu,newdata=car.test.frame)}$ | | | | | | |
| > plot(Mileage,p) | | | | | | |
| <pre>> identify(Mileage,p,label=abbreviate(row.names(car.test.frame)))</pre> | | | | | | |

We can try to look for the influential observations in the plot of observed vs predicted. When we type identify(...) we are calling an interactive procedure; now S expects us to point at the points in the graph and click on the left mouse button. It will then label the point with the vector given to the label= argument. (See fig 9). Here we used abbreviate to produce a shortened version of the label. When we don't want to label any more points, we just position the cursor anywhere on the graphics window and click on the middle mouse button. S will then return a vector with the indexes of those observations labeled, which we can use to check the data.

The legend in the plot was obtained using a combination of legend and locator.

The arguments to legend are pretty easy to interpret here, except perhaps for locator(1). locator(n) is just a drawing function which will connect n points with lines as you draw them on the screen by

clicking the mouse. legend interprets locator(1) to mean to position 1 point (the top left of the box) in the place where you click the mouse. Alternatively, a vector of coordinates could have been used.

The legend function has largely be obsoleted by the key function which is more versatile. When identifying separate curves you may also want to let Hmisc's labcurve function call key for you.

11.3 Hmisc and Design High–Level Plotting Functions

Table 11.1 summarizes high–level plotting commands from Hmisc, Design, and standard S.

The Hmisc function scat1d has several options for showing the density of the raw data through a rug plot on one of the four axes or along a user-specified curve. scat1d is especially good at showing the data density for very large datasets, as it will draw a random sub-segment of each whisker or "strand" of the rug. It has an argument which allows you to place the rug plot along a curve rather than on an axis. For extremely large datasets, you may want to use the histSpike function instead (see below). By default, if $n \geq 2000$, scat1d calls histSpike automatically.

The datadensity function is a generalization of scat1d which calls scat1d for each continuous variable in a data frame and draws frequency bar plots for categorical variables. datadensity places each variable on a separate axis and writes the number of missing values to the right of each axis if there are any NAs. datadensity is a good tool for initial data inspections (see Section 3.6). Figure 11.9 shows the result of the commands

> datadensity(prostate) # prostate is on Web page

datadensity accepts a group argument which will cause tick marks for individual raw data points to be distinguished by color. This can be used to identify associations between the group variable and the other variables.

histSpike draws a "spike" histogram using by default 100 bins. This is especially useful for large datasets as such histograms can have high resolution. histSpike can also draw a kernel density plot. A useful feature of histSpike is that like scat1d it can be used to enhance an existing plot (e.g., scatter diagram) with histograms or density plots showing the marginal distribution of one of the variables plotted. These plots point inward from any of the 4 axis lines. Unlike scat1d you have to add the argument add=T to do this.

The ecdf function in the Hmisc library draws empirical cumulative distributions for either individual variables or for all variables in a data frame. For the latter case, a suitable matrix of plots is set up automatically. ecdf also accepts a group variable, so it can automatically draw multiple cdfs based on stratifying the data on categorical variables. Curves are labeled using labcurve. Here are some examples.

```
ecdf(age, group=sex)
ecdf(age, group=interaction(sex,race))
```

Empirical distribution functions have two advantages over histograms: they do not require the choice of bins, and you can overlay several distributions on the same plot. There is a trellis version of ecdf (see Section 11.4). It is easy to have ecdf call scat1d to add a rug plot to the cumulative distribution plot, or to call histSpike to add a histogram or density plot to the plot. For example, you can type ecdf(age, datadensity='rug').

Table 11.1: Non-trellis High Level Plotting Functions

| Function | Description | | |
|----------------------|---|--|--|
| barplot | vertical or horizontal bar graph | | |
| bpplot | box–percentile plots (Hmisc) | | |
| boxplot | side-by-side boxplots | | |
| contour | contour plot | | |
| coplot | separate plots of different ranges | | |
| datadensity | multivariable version of Hmisc's scat1d | | |
| | displays data density for all variables in a data frame | | |
| dotchart | displays values based on position of dots | | |
| ecdf | empirical distribution function plot (Hmisc) | | |
| faces | Chernoff faces for multivariate data | | |
| hist | histogram | | |
| hist.data.frame | histrogram of all variables in a data frame (Hmisc) | | |
| histSpike | high–resolution "spike" histograms and density plots | | |
| labcurve | draw and label curves or label existing curves (Hmisc) | | |
| nomogram | nomograms (Design) | | |
| pairs | all possible pairs of scatterplots | | |
| persp | 3-D perspective plots of grids | | |
| pie | pie charts | | |
| plclust | plots of cluster trees from hclust | | |
| plot | scatterplot or line plot | | |
| plot.anova.Design | Dot chart of anova table (Design) | | |
| plot.Design | family of functions for fitted objects | | |
| plot.summary.Design | plots effect ratios and CIs (Design) | | |
| plot.summary.formula | plotting functions for summary.formula function (Hmisc) | | |
| plsmo | plot smoothed nonparametric estimates (Hmisc) | | |
| qqnorm | normal probability plot | | |
| qqplot | quantile-quantile plot | | |
| scat1d | add data density (rug plot) to plot (Hmisc enhancement of rug | | |
| survplot | survival plots (Design) | | |
| symbol.freq | diagram of frequency table (Hmisc) | | |
| tsplot | time series plots | | |
| usa | map of the US | | |

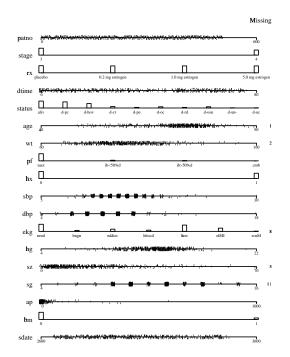


Figure 11.9: datadensity plot for the prostate data frame

The builtin function cdf.compare draws an empirical CDF alongside a theoretical one. See also the trellis stripplot function discussed in Section 11.4.

There are several builtin ways to draw box and whisker plots in S. These plots provide useful overall summaries but they are not especially sensitive to the behavior of the tails of the distributions. A continuous version of the box plot called the box-percentile plot, was developed by Esty and Banfield. Banfield's bpplot function, with slight modifications, is included in Hmisc. To quote from Banfield's help file for bpplot: "Box-percentile plots are similiar to boxplots, except box-percentile plots supply more information about the univariate distributions. At any height the width of the irregular 'box' is proportional to the percentile of that height, up the the 50th percentile, and above the 50th percentile the width is proportional to 100 minus the percentile. Thus, the width at any given height is proportional to the percent of observations that are more extreme in that direction. As in boxplots, the median, 25th and 75th percentiles are marked with line segments across the box".

The leftmost arguments to **bpplot** may be a sequence of not necessarily equal-length vectors or a list containing the same. The latter is often produced by the **split** function in order to stratify on a grouping variable.

Here is an example of a box-percentile plot showing the distribution of ages in the titanic data frame, stratified by passenger class. We add a group representing the overall age distribution and a hypothetical group having a normal distribution with the same mean and variance of the overall age distribution. To omit these extra groups use the simple command bpplot(split(age,pclass), xlab='Passenger Class', ylab='Years').

The result is shown in Figure 11.10.

Hmisc's labcurve function will automatically label a set of existing curves on the current plot, or draw and label curves, if you tell it the coordinates of all of the curves. labcurve has many options. By default it will label curves at the points for which they are maximally separated. You can usually get away without a legend if you do this. If you want a legend, labcurve will position the legend at the most empty area of the plot, and it is easier to use than the key or legend commands in many cases. Here is an example where labcurve draws and labels the curves. The lines are distinguished by different colors and styles.

The plsmo function plots smoothed estimates of x vs. y, handling missing data for lowess or supsmu, and adding axis labels. It optionally suppresses plotting extrapolated estimates. An optional group variable can be specified to compute and plot the smooth curves by levels of group. When group is present, the datadensity option will draw tick marks showing the location of the raw x-values, separately for each curve. plsmo also has an option to plot connected points for raw

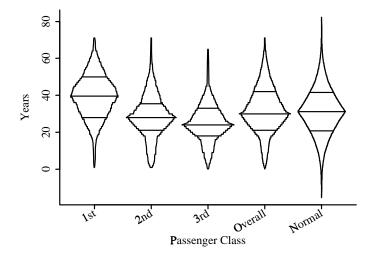


Figure 11.10: Box-percentile plot showing the distribution of ages of passengers on the Titanic stratified by passenger class. More than half of the passengers are omitted from this plot due to missing ages. The rightmost part of the plot shows the box-percentile plot for a normal distribution having mean and standard deviation equal to that of the ages in the data.

data, with no smoothing. Here is an example in which the log odds of smoothed estimates of the probability of death vs. age is plotted, stratified by sex.

plsmo(age, death, group=sex, datadensity=T, fun=plogis)

See also the Hmisc trellis panel function panel.plsmo described in Section 11.4.

11.4 trellis Graphics

S-PLUS also comes with a library of advanced graphics functions called trellis. In R, this library is called lattice. The library name comes from the fact that when you are displaying multiple graphics panels after conditioning on other variables, the resulting display looks like a garden trellisor lattice. trellis has these advantages over S's older graphical functions:

- 1. trellis uses better defaults for fonts, colors, and point symbols.
- 2. It uses S symbolic formulas for specification of the main and conditioning variables.
- 3. Related to the last point, you can condition on one variable or on the cross-classifications of any number of "given" variables.
- 4. Some new graphics types are implemented, including some for 3–D plots.
- 5. Graphical parameters such as the aspect ratio are chosen for improved graphical perception.

| Function | Purpose | Formula Argument |
|---------------------|--|-----------------------------|
| barchart | Bar chart | y ~ x g1*g2 |
| bwplot | Box and whisker plot | y ~ x g1*g2 |
| densityplot | Probability density plot | ~ x g1*g2 |
| dotplot | Dot plot | y ~ x g1*g2 |
| Dotplot | Hmisc generalization of dotplot | y ~ x g1*g2 |
| ecdf | Hmisc ECDF plot | ~ x g1*g2, |
| | | groups=g3 |
| histogram | Histogram | ~ x g1*g2 |
| parallel | Parallel coordinate plot | ~ x g1*g2 |
| panel.bpplot | enhanced box plots and | |
| | box-%-tile plots with bwplot | |
| panel.plsmo | Hmisc panel function for | y ~ x g1*g2, |
| | xyplot | groups=g3 |
| splom | Multi–panel scatterplot matrices | ~ x g1*g2 |
| stripplot | One–dimensional scatter plot | y ~ x g1∗g2 |
| xyplot | Conditioning plots/scatter plots | y ~ x g1*g2 |
| xYplot | Hmisc generalization of xyplot | Cbind(y,y2,y3) ~ x g1*g2, |
| | for multi–column y | groups=g3 |
| setTrellis | Hmisc trellis setup | |
| trellis.strip.blank | Hmisc function to set trellis | |
| - | to use blank background for panel titles | |

Here is a list of some of the most commonly used trellis functions.

Type ?trellis to see several other trellis functions. In the formulas, g1,g2,g3 are categorical "given" (conditioning) variables. There may be more than two of them. If only one is given, the *s are omitted. y is a factor variable (except for xyplot for which it is numeric), and x is a numeric variable. For splom, x is a matrix or a data frame. parallel is useful for representing multivariate data. For it, x is a numeric matrix whose columns represent the multivariate response. See Section 11.4.1 for a generalization of xyplot in Hmisc.

You can use trellis's shingle function to make overlapping intervals of a continuous variable, to use it as a conditioning or y variable. The equal.count function is convenient for this. For example, the g1, g2 variables above could be of the form equal.count(z) where z is a numeric continuous variable. Optional arguments to equal.count are number (number of intervals) and overlap (degree of overlap between intervals). Defaults are 6 and .5, respectively.

When plotting a factor variable, particularly when making dot plots, one frequently wants to control the ordering of factor levels in constructing an axis or in arranging panels. The **reorder.factor** function is useful for this. As an example consider two simple vectors. For generality, we create a factor variable whose levels are not in alphabetic order.

```
> a ~ c(1, 3, 2.5, 2.2)
> b ~ factor(c('a', 'c', 'b', 'd'), c('d', 'c', 'b', 'a'))
levels(b)
[1] "d" "c" "b" "a"
> dotplot(b ~ a)  # y-axis is a b c d (from bottom to top)
> # Now re-order levels of b to be in order of a
> b ~ reorder.factor(b, a)
> b
[1] a c b d
> levels(b)
[1] "a" "d" "b" "c"
> dotplot(b ~ a)  # y-axis is a d b c (bottom to top)
```

This places the dots in ascending order from bottom to top. To put them into descending order, use instead

> b \leftarrow reorder.factor(b, -a)

You can also order factor levels by another variable, and if the data are not already grouped, by the value of a summary statistic computed after grouping. **reorder.factor** creates an ordered variable and trellis functions respect the order of the levels of such variables (see the **ordered** function).

Most of the trellis functions accept a groups argument that is used in conjunction with the panel.superpose function to plot different classes of points in the same plot (superposition), distinguishing them by different symbols or colors. For example, to plot age vs. height on one plot using different color symbols for females and males we might use the command

<code>xyplot(height</code> \sim <code>age, groups=sex, panel=panel.superpose)</code>

This can be enhanced by allowing the user to control the plotting symbols and other characteristics. In what follows we plot males using an x (pch=2) and females using a triangle (pch=4). We use the key option to place a legend on top of the plot.

If you want the key to have one row, specify columns=2 inside the key list.

By combining trellis' xyplot function with Hmisc's panel.plsmo function, more flexibility is obtained and keys can be created to define multiple groups of data points on one trellis panel. By default, both raw data and nonparametric trend estimates are graphed. The previous example could be done using

```
xyplot(height \sim age, groups=sex, panel=panel.plsmo, type='p') Key()
```

Here type='p' caused only points to be drawn. The default, type='b' causes both raw data points and lowess-smoothed trend lines to be drawn, and the different curves are labeled by the group names where the curves are furthest apart. Specify type='l' to omit the raw data points.

Here are some other examples:

The Key function is created by panel.plsmo when a groups variable is present. Key calls the builtin key function with suitable arguments for drawing the key, remembering what was specified to xyplot in the form of symbols and colors.

Here are some other trellis examples.

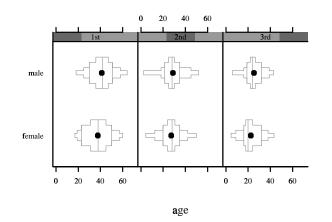


Figure 11.11: Extended box plot for titanic data. Shown are the median, mean (solid dot), and quantile intervals containing 0.25, 0.5, 0.75, and 0.9 of the age distribution.

```
# Add datadensity='rug', 'hist', or 'density' to augment CDF with
# density information
library(Design,T); attach(prostate) # prostate is on web page
x ← nomiss(cbind(age,wt,sbp,dbp,hg,sz))
# Using nomiss in Hmisc - splom has a bug in handling missing values
splom(~ x)
```

trellis shades panels which label the current level of conditioning variables. To instead use white backgrounds on these title panels, use the following commands:

```
s.b ← trellis.par.get("strip.background")
s.b$col ← 0
trellis.par.set("strip.background", s.b)
s.s ← trellis.par.get("strip.shingle")
s.s$col ← 0
trellis.par.set("strip.shingle", s.s)
```

This can be also be done by using the command trellis.strip.blank(), which calls a little function in Hmisc. trellis.strip.blank must be called before the graphics device is opened. Another way to remove shading from the strip is to add the following argument to a top-level trellis function:

```
strip=function(...) strip.default(..., style=1)
```

The help file for strip.default documents the various values of style:

1. the full strip label is colored in background color and the text string for the current factor level is centered in it

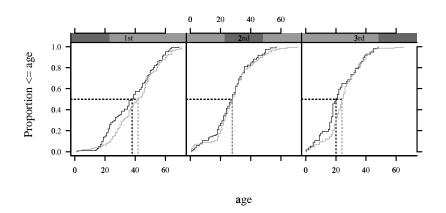


Figure 11.12: Multi-panel trellis graph produced by the Hmisc ecdf function.

- 2. all the factor levels are spread across the strip with the current level is drawn atop a colored rectangle
- 3. identical to style 1 but a portion of the strip is highlighted (as in a shingle) to indicate the position of the current level
- 4. like 2 except the entire strip label is colored in background color
- 5. like 1 but the current factor level is positioned left-to-right across the strip
- 6. like 5 but the string adjustment varies from left-justified to right-justified as the string moves left-to-right

The Hmisc setTrellis function by default calls trellis.strip.blank and sets the line thickness for dot plot reference lines to 1 instead of the usual default of 2. See also the setps Hmisc function.

For Lattice graphics under R, the best way to set up for black and white graphics with transparent strip backgrounds is to use the following commands at the top of the program.

```
library(lattice)
ltheme <- canonical.theme(color = FALSE)
ltheme$strip.background$col <- "transparent"
lattice.options(default.theme = ltheme)</pre>
```

There are many standard options to high-level trellis functions (a good reference is Kraus & Olson Section 6.4). If you are making a multi-panel graph that is 2 rows \times 2 columns with one of the four panels unused, you can specify that all 3 panels are to be put in a row. Add layout=c(1,3) to put then in one row or layout=c(3,1) to put the three panels in one column. You can specify a logical vector skip to control where unused panels appear. To make a 2 \times 2 layout with the upper

left panel being blank, specify layout=c(2,2), skip=c(F,F,T,F); note the numbering from the origin of the lower left panel. You can arrange and number panels from the upper left by using the as.table=T argument.

Trellis graphs are not actually drawn until a **print** function is executed, either explicitly or implicitly. This can be used to great advantage in composing a multi-graph display of different types of Trellis graphs. In the following example we make four graphs and do not draw them immediately. The **print.trellis** is invoked to put the four graphs in the desired locations on the page.

The first two arguments to **split** specify the column and row number (from the lower left) the current graph should occupy. The last two arguments specify the overall number of columns and rows that are to be set aside.

To have finer control of positioning of sub-graphs you can use the **position** argument which contains fractional values. For details see the help file for **print.trellis**.

To specify axis details, use scales=. For example, to specify that 10 tick marks are to appear on the x-axis and 5 on the y-axis, use scales=list(x=list(tick.number=10),y=list(tick.number=5)).

Specify aspect='xy' to bank panels to 45° .

See the trellis.args help file for more information about general trellis arguments including main, sub, page, xlim, ylim, xlab, ylab. To graphically display all the current trellis settings, issue the show.settings() command.

When you want to display the data density of one variable stratified by one or more other variables and you don't like cumulative distribution functions or multiple histograms, the trellis stripplot function may be of interest, as a generalization of Hmisc's datadensity function (Section 11.3). By default, stripplot makes a separate horizontal band for each level of the stratification variable and plots small circles at each actual data point (with optional jittering). You can give stripplot a panel argument to specify other representations. Here are some examples:

```
lines(d$x, d$y + yy)
}
stripplot(treatment ~ y, panel=g)
```

A much easier approach to producing the previous graph is to use the **trellis densityplot** function as shown below. A second example uses the **prostate** data frame that is in the Design library.

```
densityplot(~ y | treatment)
densityplot(~hg | rx*factor(stage), width=3, data=prostate)
```

See Section 6.1 for an example where a frequency table is constructed for two categorical variables, row percents are computed, and these are plotted using dotplot.

You can find out more about trellis by visiting MathSoft's Web page http://www.mathsoft.com/splus.html.

11.4.1 Multiple Response Variables and Error Bars

The trellis xyplot function is quite flexible as long as you are plotting a single response variable. Trellis in general requires the response variable to be univariate so there is no opportunity to add, for example, a systolic blood pressure time trend to a diastolic pressure trend on the same panels. There is also no way with xyplot of plotting "error bars" such as mean ± 2 standard errors, or the median and outer quartiles. Hmisc's xYplot function uses a trick to get around this problem. The trick is that the analyst specifies multiple response variables, but all but the first are converted to become attributes of the first variable, using an auxiliary function Cbind. Then a new panel function panel.xYplot fetches these attributes as needed.

xYplot other advantages over xyplot.

- 1. It automatically goes into "superpose" mode when a groups variable is present. No panel = panel.superpose needs to be specified.
- 2. xYplot produces a function Key that makes it easy to plot a key for how the groups variable is denoted in the plot.
- 3. xYplot can use the Hmisc labcurve function to automatically label multiple curves generated by the groups variable.
- 4. xYplot uses variable labels, when they are present, to label axes.
- 5. xYplot can aggregate raw data automatically, given a function that produces a 3-number summary. Numeric x-variables can be collapsed into intervals containing a pre-specified number of observations, and represented by the mean x within the intervals.

Here are some examples taken from the help file. The first several examples draw error bars, then other examples show how to plot multiple curves generated by the multiple response variables, using e.g. method='band'. For any plot, you can control whether lines or points are plotted through the use of type='l', 'p', or 'b' (both).

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```
# First generate combinations of some variable values
dfr \leftarrow expand.grid(month=1:12, continent=c('Europe', 'USA'),
                   sex=c('female','male'))
attach(dfr) # to get access to 3 new variables
set.seed(13) # so values can be replicated
# Add a response variable (monthly mean) to the predictor settings
# using an assumed linear regression model
y <-- month/10 + 1*(sex=='female') + 2*(continent=='Europe') +
    runif(48,-.15,.15)
lower \leftarrow y - runif(48,.05,.15)
                                 # Generate hypothetical monthly ranges
upper \leftarrow y + runif(48,.05,.15)
# Show mean and range at each month, for one panel
xYplot(Cbind(y,lower,upper) ~ month,subset=sex=='male' & continent=='USA')
# add ,label.curves=F to suppress use of labcurve to label curves where farthest apart
# Now make a panel for each continent, for males
xYplot(Cbind(y,lower,upper) ~ month|continent,subset=sex=='male')
# Make a panel for each continent; within each panel, separate sex
# groups; use Key to automatically place a key
xYplot(Cbind(y,lower,upper) \sim month|continent,groups=sex); Key()
# Separate sex groups within a single panel
xYplot(Cbind(y,lower,upper) ~ month,groups=sex,subset=continent=='Europe')
# Same as above but automatically position labels for sex groups
xYplot(Cbind(y,lower,upper) ~ month,groups=sex,subset=continent=='Europe',keys='lines')
# keys='lines' causes labcurve to draw a legend where the panel is most empty
# Draw 3 lines for the three variables
xYplot(Cbind(y,lower,upper) \sim month,groups=sex,subset=continent=='Europe',method='bands')
# Show error bars once again, but only the upper part
xYplot(Cbind(y,lower,upper) \sim month,groups=sex,subset=continent=='Europe',method='upper')
# Now use a label for y, and alternate using only upper or lower bars
# so bars for different groups don't run into each other
label(y) \leftarrow 'Quality of Life Score'
# can also specify Cbind('Quality of Life Score'=y,lower,upper)
xYplot(Cbind(y,lower,upper) \sim month,groups=sex,subset=continent=='Europe',method='alt bars',
       offset=.4) # offset passed to labcurve to label .4 y units away from curve
```

In the standard R Lattice package you can add error bars to plots with xyplot by passing an auxiliary variable and using the subscripts of the data being plotted in the current panel¹:

> xyplot(y ~ x, data, sd = data\$sd, + panel = function(x, y, subscripts, sd, ...) { + larrows(x, y - 2 * sd[subscripts], 235

¹This example was provided by Deepayan Sarkar.

```
+ x, y + 2 * sd[subscripts],
+ angle = 90, code = 3, ...)
+ panel.xyplot(x, y, ...)
+ })
```

11.4.2 Multiple *x*-axis Variables and Error Bars in Dot Plots

The Hmisc Dotplot function has three of the four advantages over the builtin trellis function dotplot that xYplot has over xyplot. But instead of generalizing the function to allow multiple y-axis variables, Dotplot generalizes dotplot to allow for several x-axis variables. The main usage of this is displaying confidence or quantile intervals on the horizontal reference lines, in addition to showing point estimates. For example, to turn the last xYplot example into a dot plot, use

This will produce a solid line² connecting the lower and upper values for each month, with a solid dot indicating the value of y. To further emphasize the range rather than the point estimate, specify pch=3 (plus sign) as the plotting symbol.

Like dotplot, panel variables can be used with Dotplot when the formula contains a |. Dotplot does not fully handle both superposition (using groups) and multiple x-variables, as it currently does not use different colors or other line styles to distinguish the low-high line segments for the superposed groups.

See Section 4.8 for examples where Dotplot is used for profiling multiple groups, based on means, confidence limits, and ranks.

11.4.3 Using summarize with trellis

The Hmisc summarize function creates a new data frame containing multi-way descriptive statistics. This data frame is suitable for use by all trellis functions. In the next example we generate a dataset containing $24 \text{ month} \times \text{year}$ combinations with 100 observations per combination. Then we compute 24 medians and 0.025 and 0.975 quantiles to show the center and 0.95 coverage intervals for each stratum.

```
keys='lines', method='alt')
```

²The line style is taken from trellis.par.get('plot.line').

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month year y Lower Upper 1 1997 6.55 6.44 6.67

```
1 1998 7.51 7.40 7.62
    2 1997 5.58 5.47 5.69
    2 1998 6.44 6.33 6.55
    3 1997 4.53 4.42 4.67
    3 1998 5.47 5.37
                      5.58
    4 1997 3.36 3.26
                      3.46
    4 1998 4.59 4.49
                      4.69
    5 1997 2.48 2.36 2.60
    5 1998 3.31 3.22 3.41
    6 1997 1.58 1.47 1.69
    6 1998 2.50 2.38 2.60
    7 1997 1.39 1.28 1.51
    7 1998 2.47 2.36 2.58
    8 1997 2.54 2.43 2.64
    8 1998 3.43 3.32 3.55
    9 1997 3.52 3.42 3.63
    9 1998 4.56 4.45 4.67
   10 1997 4.50 4.39 4.63
   10 1998 5.52 5.41 5.62
   11 1997 5.49 5.37
                      5.61
   11 1998 6.44 6.34 6.56
   12 1997 6.51 6.39 6.64
   12 1998 7.47 7.37 7.58
xYplot(Cbind(y, Lower, Upper) \sim month | year, data=s)
```

To convert this to a dot plot, use

<code>Dotplot(month</code> \sim <code>Cbind(y, Lower, Upper)</code> | year, data=s, pch=3)

The combination of summarize and trellis graphics is also useful for showing empirical results when the number of points is too large to make an interpretable scatterplot (especially when stratified by categories of a third variable). In what follows we compute the three quartiles of height stratified by age and sex simultaneously. We either round age to the nearest year, or group it into deciles, to have sufficient sample sizes in each age × sex stratum. For grouping age into deciles, we use a feature of the Hmisc cut2 function in which the levels for the decile groups are the mean values of age within each decile group. We have to go to extra trouble to convert the factor variable created by cut2 to a numeric variable.

```
ageg ← round(ageg) # or:
ageg ← as.numeric(as.character(cut2(age,g=10,levels.mean=T)))
```

This process has been automated in xYplot:

```
xYplot(height \sim age, groups=sex, method='quantiles')
```

Here method='quantiles' runs cut2 and summarize on the raw data to produce the summarized data. By default, this will, for each sex, group age into intervals containing min(40, n/4) observations where n is the number of observations in that sex group. You can override this using the nx argument to xYplot. You can also specify the vector of 3 quantiles to compute, in a probs argument. The central quantile needs to be listed first. method can also be the name of a function that returns a matrix containing, in order, a measure of central tendence and some sort of limits. For example:

xYplot(y \sim month | year, nx=F, method=smean.cl.boot)

displays the mean y and bootstrap confidence limits, stratified by unique values of month (with no intervals, because nx=F was specified). You can specify instead nx=m where m is the number of observations to achieve in each automatically-created x interval.

See Section 6.1 for an example where row percentages are computed from a frequency table, and then displayed using trellis graphics. Section 4.8 has other examples for summarize and Dotplot.

If the data frame is organized so that the multiple variables to plot are in separate rows, the Hmisc reShape function may be useful for reorganizing the data for plotting. Here is an example where for each Department there is a row for each of three salary levels: low, middle, and high. A variable named type tells what each row pertains to. reShape will create a matrix with columns named low,middle,high. Here we assume the levels of type are in the order middle, low, high. indexhlabel

```
label(salary) ← 'Salary, $'
a ← reShape(salary, id=Department, colvar=type)
dept ← dimnames(a)[[1]]
Dotplot(dept ~ Cbind(a))
```

Note that when there is a single argument to Cbind and that argument is a matrix, Cbind will pull off the first column as the main variable and "hide" the other columns as an attribute to the main variable.

11.4.4 A Summary of Functions for Aggregating Data for Plotting

Various functions in S can be used to compute aggregate statistics with stratification that can be passed to various plotting routines. A summary of these functions is below.

tapply: This function will stratify a single variable by one or a list of stratification variables. When you stratify by more than one variable, the result is a matrix which is generally difficult to plot directly. The Hmisc reShape function can be used to re-shape the result into a data frame for plotting. When you stratify by a single variable, tapply creates a vector of summary statistics suitable for making a simple dot or bar plot without conditioning.

- aggregate: The function takes as input a vector or a data frame and a by list of one or more stratification variables (see p. 89). It is handy to enclose the by variables in the llist function. You can summarize many variables at once but only a single number such as the mean is computed for each one. aggregate does not preserve numeric stratification variables — it transforms them into factors which are not suitable for certain graphics. The result of aggregate is a data frame for printing or plotting.
- summary.formula: This Hmisc function by default will compute separate summaries for each of the stratification variables. It can also do cross-classifications when method='cross'. You can summarize the response variable using multiple statistics (e.g., mean and median) and if you specify a fun function that can deal specially with matrices, you can summarize multiplecolumn response variables. summary.formula creates special objects and has special plotting methods (e.g., plot.summary.formula.response) for plotting those objects. In general you don't plot the results of summary.formula using one of the trellis functions.
- summarize: This Hmisc function has a similar purpose as aggregate but with some differences. It will summarize only a single response variable but the FUN function can summarize it with many statistics. Thus you can compute multiple quantiles or upper and lower limits for error bars. summarize will not convert numeric stratifiers to factors, so summarize is suitable for summarizing data for xyplot or xYplot when the stratification variable needs to be on the *x*-axis. summarize only does cross-classification. It will not do separate stratifications as the summary.formula function does. Unlike summary.data.frame, summarize creates an ordinary data frame suitable for any use in S, especially for passing as a data argument to trellis graphics functions. You can also easily use the GUI to graph this data frame.
- method=function with xYplot: This automatically aggregates data to be plotted when central tendency and upper and lower bands are of interest.

Chapter 12

Controlling Graphics Details

S has the capabilities to produce very complex and detailed graphical summaries. Loosely speaking, there are three levels of complexity in the elements comprising a plot. The first level consists of commands that can produce a plot by themselves. They set up a coordinate system for us and automatically determine the size of the plot, margins, orientation, font, plotting characters and the box surrounding the plot. They are called *high level* plotting functions. They can be described as functions that will produce results with a single call to them. Examples of high level plotting functions include plot, hist and boxplot. The next level allows to add detail to the plot by including other elements such as lines, symbols, legends, draw polygons, etc. These kind of functions are called *low level* plotting functions. They are functions whose output is added to a currently active graphics device. Finally, the greatest detail and control over your graphics can be exercised through the use of graphics parameters. Others can be used in high level plotting functions; they are called *high level parameters*. There are also *layout parameters* which can only be changed through par because they change the overall layout of plots or figures. The last category of parameters are *information parameters* which cannot be changed but can be queried through par.

Table 12.1 summarizes low–level plotting commands for taking charge of details of how plots are drawn.

The undocumented Hmisc function pstamp uses the stamp function to date/time stamp an existing plot or multi-image plot. Under UNIX, pstamp can optionally stamp the plot with the current project directory name. Additional user-specified text (the first argument) can be specified; this is used as a prefix to the stamp. Unlike stamp, pstamp uses very small letters so as to not obstruct the rest of the graph.

12.1 Graphics Parameters

The function **par()** with no arguments returns a list. We list below the names of all the parameters in alphabetical order. In order for **par()** to work, a graphics device should be active.

 Table 12.1: Low Level Plotting Functions

| Function | Description |
|-----------------|--|
| abline | add straight line to plot |
| arrows | draw arrow |
| axes | add axis label |
| axis | add custom axis |
| box | add box to plot |
| character.table | show special text symbols (Hmisc) |
| frame | advance to next figure |
| labelclust | add labels to cluster plot |
| legend | add legend to plot |
| lines | add lines |
| minor.tick | add minor tick marks (Hmisc) |
| mtext | add text in margins |
| mtitle | add titles and subtitles to a multiple image plots (Hmisc) |
| perspp | project points on perspective plots |
| points | add points |
| polygon | draw and shade polygons |
| pstamp | date/time stamp current plot (Hmisc enhancement of stamp) |
| qqline | draw median line on qqnorm plot |
| rug | add data-based marks to an axis |
| segments | draw disconnected line segments |
| show.pch | show plotting characters (Hmisc) |
| stamp | add a time stamp to a plot |
| symbols | draw symbols on a plot |
| text | add text |
| title | add title or axis labels |

> names(par()) [1] "1em" "adj" "ask" "bty" "cex" "cin" "col" "cra" "crt" "csi" "fig" [11] "cxy" "din" "err" "exp" "fin" "font" "frm" "fty" "lab" [21] "las" "ltv" "lwd" "mai" "mex" "mar" "mfg" "mgp" "new" "oma" [31] "omd" "omi" "pch" "pin" "plt" "pty" "rsz" "smo" "tck" "srt" [41] "uin" "usr" "xaxp" "xaxs" "xaxt" "xpd" "yaxp" "yaxs" "yaxt"

To change one or more of the parameters we pass them to **par** as arguments with their new values. For instance, to change the default plotting symbol from "*" to "+" and setup a matrix of plots with two rows and three columns, we would type

> par(mfrow=c(2,3),pch=3)

The statements above, did not only change the value of mfrow and pch but also returned *invisibly* a list containing the original values of the parameters that we changed. Thus, if we were going to assign the statement, we would get a list with these original values. This can be useful to restore the parameters to its previous values.

```
> par.old ← par(mfrow=c(2,3),pch=3)
> par.old
$mfrow:
[1] 1 1
$pch:
[1] "*"
> par(par.old)
> par()$mfrow
NULL
> par()$pch
[1] "*"
```

The value of some parameters may change when you change another. The parameter cex for example, which controls character expansion relative to the device size, is related to the mfrow parameter. When you change mfrow, cex will be set automatically, so that the character size is not too big for the number of plots in the screen. You can still change cex to be whatever you like. You just have to do it after you set mfrow and in a different par. The reason for doing it in a different par is that cex is a general graphics parameter and mfrow is a layout parameter. S sets general parameters first and then layout parameters.

```
> par(mfrow=c(3,2))
> par(cex=0.75)  # NOT par(mfrow=c(3,2),cex=0.75)
```

12.1.1 The Graphics Region

To understand what each parameter does it is necessary to visualize how S divides up the device surface. We have an *outer margin*, inside of which we find the *figure region*. This region contains one or more *plot areas* surrounded by a *margin*.

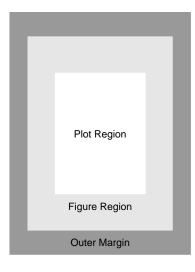


Figure 12.1: Plot Region

By default the device is initialized with zero area in the outer margin. Typically the axis line is drawn in the border between the plot region and the margin. If we change the size of one of the regions, the others are adjusted automatically.

12.1.2 Controlling Text and Margins

The parameters to control the size of the outer margin are oma,omi and omd. For the figure margin we use mar and mai. Related to all of them is mex. The parameters fig and fin control the physical size of the figure region, while plt and pin do likewise for the plot region. Here is a description of all of them

```
fig=c(x1,x2,y1,y2)
            coordinates of the current figure region expressed as a
            fraction of the device surface. This is dependent on
            mfrow and mfcol.

fin=c(w,h)
            width and height of figure in inches.

mai=c(xbot,xlef,xtop,xrig)
            margin size specified in inches. Values given for bottom,
            left, top, and right margins in that order.

mar=c(xbot,xlef,xtop,xrig)
            lines of margin on each side of plot. Margin coordinates
```

range from 0 at the edge of the box outward in units of mex sized characters. If the margin is respecified by mai or mar, the plot region is re-created to provide the appropriate sized margins within the figure. The default value is c(5,4,4,2)+.1. Problems with lines not appearing on some devices might be remedied by specifying non-integer values in mar.

mex=x the coordinate unit for addressing locations in the margin is expressed in terms of mex. Margin coordinates are measured in terms of characters of size cex equal to mex. mex does not change the font size - it merely states which font is to be used to measure the margins.

```
oma=c(xbot,xlef,xtop,xrig)
```

outer margin lines of text. oma provides the maximum value for outer margin coordinates on each of the four sides of the multiple figure region. oma causes recreation of the current figure within the confines of the new-ly specified outer margins. The default is rep(0,4). See mtext to create titles in the outer margin.

```
omd=c(x1, x2, y1, y2)
```

coordinates of the outer margin region as a fraction of the device surface.

omi=c(xbot,xlef,xtop,xrig)
 size of outer margins in inches.

pin=c(w,h)

width and height of plot, measured in inches.

```
plt=c(x1,x2,y1,y2)
    the coordinates of the plot region measured as a fraction
    of the figure region.
```

By default we start with zero area for the outer margin. We can change it by changing oma, omd or omi. It is easiest to work with oma since it measures relative sizes; namely, the number of lines of text that we want to have in the outer margin. The height of the lines is measured in units of mex which is just the size of the default font. Thus if oma is c(0,0,5,0) and mex has the default value of one, it means that we are leaving room for zero lines of text in the bottom, right and left margin and 5 lines of text of the default size at the top. This does not mean that the text itself that we type has to be of the default size. The size of text is determined by the value of cex (character expansion). If cex equals 2.5, then we can only fit two lines of text at the top. Of course changing oma changes some of the other parameters. The physical size of the figure and plot regions will be reduced. However the space for margins in the figure region will remain the same.

Let us look at an example. We list below the default values of the parameters mentioned above.

> par(Cs(fig,fin,mai,mar,mex,cex,oma,omd,omi,pin,plt))
\$fig:

```
[1] 0 1 0 1
$fin:
[1] 8.00 6.32
$mai:
[1] 0.714 0.574 0.574 0.294
$mar:
[1] 5.1 4.1 4.1 2.1
$mex:
[1] 1
$cex:
[1] 1
$oma:
[1] 0 0 0 0
$omd:
[1] 0 1 0 1
$omi:
[1] 0 0 0 0
$pin:
[1] 7.132 5.032
$plt:
```

Now, let us change the value of oma to allow space for 5 lines of text in the default size of the default font (mex=1).

```
> par(oma=c(0,0,5,0))
> par(Cs(fig,fin,mai,mar,mex,cex,oma,omd,omi,pin,plt))
$fig:
[1] 0.0000000 1.0000000 0.0000000 0.8892405
$fin:
[1] 8.00 5.62
$mai:
[1] 0.714 0.574 0.574 0.294
$mar:
[1] 5.1 4.1 4.1 2.1
$mex:
```

[1] 0.0717500 0.9632500 0.1129747 0.9091772

246

```
[1] 1
$cex:
[1] 1
$oma:
[1] 0 0 5 0
$omd:
[1] 0.0000000 1.0000000 0.0000000 0.8892405
$omi:
[1] 0.0 0.0 0.7 0.0
$pin:
[1] 7.132 4.332
$plt:
[1] 0.0717500 0.9632500 0.1270463 0.8978648
```

We see that all the parameters have changed with the exception of mai, mar, mex and cex. Let us now change mar and cex to allow for only one line of text of size 2.5 in the top margin figure.

```
> par(mar=c(0,0,2.5,0))
> par(cex=2.5)
> mtext("A Title in the Figure Margin",side=3)
> mtext("A Title in the Outer Margin",side=3,outer=T,line=2.5)
> mtext("Another Title in the Outer Margin",side=3,outer=T)
> text(0.5,0.5,"This is the qPlot Region",cex=1)
> box()
```

Look at the help file for an explanation on the use of mtext. Also notice that we used text with a pair of coordinates despite the fact that there was no plot in the graphics surface. The reason we could do this is that S sets up a coordinate system as soon as you open a graphics device. The default coordinates are c(0,1,0,1) as determined bypar("usr"). If we were going to issue a high level plotting command this coordinates would be set according to the range of your data.

One other layout command that we can look at is pty. The value of pty is a character string: "s" for a square plotting region, and "m" for a maximal region.

12.1.3 Controlling Plotting Symbols

We can specify the type of line to be used and its width with the parameters lty and lwd. The plotting symbol used by default is a ".". We can change it to any character we want by specifying pch="c", where "c" is any character. We may also use a number from 0 to 18 instead of a character to obtain a variety of symbols. Other numbers up to 252 yield characters that are font and device dependent as explained in the section of the help file below. If we use a character as a plotting symbol its size will be determined by the value of cex just as in the case of text. If we use a special symbol (by using the pch=n form) the size of the symbol will be given by mkh. The value of mkh is a non-negative number giving the height in inches of the symbol. A value of zero for mkh (the default) means that the symbol will be of approximately the same size as a capital letter according to cex.

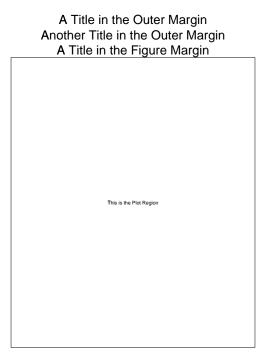


Figure 12.2: Handling text in margins

- lty=x line type, device dependent. Normally type 1 is solid, 2 and up are dotted or dashed. A few devices have only one line type.
- lwd=x line width, device dependent. Width 1 is the standard width for the device. Many devices cannot change line width.
- mkh=x height in inches of mark symbols drawn when pch is given as a number. The default value of 0 means that the cex parameter controls the size of symbols when pch is a number (the symbol is approximately the size of a capital letter in this case).
- pch="c" the character to be used for plotting points. If pch is a period, a centered plotting dot is used.
- pch=n the number of a plotting symbol to be drawn when plotting points. Basic marks are: square (0); octagon (1); triangle (2); cross (3); X (4); diamond (5) and inverted triangle (6). To get superimposed versions of the above use the following arithmetic(!): 7==0+4; 8==3+4; 9==3+5; 10==1+3; 11==2+6; 12==0+3; 13==1+4; 14==0+2. Filled marks are square (15), octagon (16), triangle (17), and diamond (18). Use the mkh graphics parameter to control the size of these marks. See the EXAMPLES section for a display of the plotting symbols. Using the numbers 32 through 126 for pch yields the 95 ASCII characters from space through tilde (see the SPLUS data set font). The numbers between 161 and 252 yield characters, accents, ligatures, or nothing, depending on the font (which is device dependent).

You may use the code below to produce a graph of the different plotting symbols and line types, then print a copy to have as a reference. Then you could do something similar to look at the effects of changing the mkh and lwd parameters.

```
> # A comprehensive pch table can be obtained using the Hmisc show.pch function
> par(usr=c(-1,19,0,1))
> for(i in 0:18)
> points(i,.5,pch=i)
> text(i,.35,i)
> title('Samples of "pch=" Parameter')
> box()
> par(usr=c(-1,11,0,11))
> for(i in 1:10)
> abline(h=i,lty=i)
> text(5,i+.5,paste("lty=",i,sep=""))
> box()
> title('Examples of "lty"')
```

The Hmisc character.table function written by Pierre Joyet shows the numeric equivalents of all latin characters, facilitating the use of special characters in graph titles and other character

Samples of "pch=" Parameter

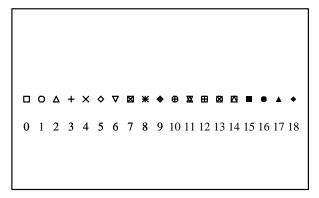


Figure 12.3: Plotting Symbols

Examples of "lty"

| lty=10 |
|--------|
| lty=9 |
| lty=8 |
| lty=7 |
| lty=6 |
| lty=5 |
| lty=4 |
| lty=3 |
| lty=2 |
| lty=1 |
| |

Figure 12.4: Different Types of Lines

strings. Typing character.table(8) for example will show the characters in font 8. From that you will see that ρ is equivalent to 162. So title('\162', font=8) will write a title of ρ .

12.1.4 Multiple Plots

To construct a plot with several figures in it we use the parameters mfrow=c(m,n) or mfcol=c(m,n). These set up a matrix of plots with m rows and n columns and the plots are drawn row-by-row or column-by-column. Setting one implies setting the other, to the same value. To know the order in which to do the plots, S looks at fty which will have the value "r" (rows) or "c" (columns) depending on which parameter was set. If the number of rows or columns is greater than 2 then cex and mex are set to 0.5.

12.1.5 Skipping Over Plots

We will now examine the function frame. We can use it to cause the graphics driver to advance to the next frame, that is, the next plot. If we have only one plot per page, the command frame() will erase the current plot (because it is moving to the next frame). In a multiple figure layout, a call to frame will move to the next figure. This provides an alternative way to skip over one or more plots in the layout. Two successive calls to frame will skip over the next figure.

The parameter **new** on the other hand, is a logical parameter whose purpose is to determine whether or not a high level function will move to the next figure or overlay the current one. If **new=T** it is assumed there are no plots in the current figure and therefore the canvas *will not* be erased when we call a high level function. If **new=F** then a call to a high level function will cause the graphics device to move to the next figure in order to avoid overwriting the current one. After executing a high level graphics command **new** is immediately set to F. This the normal situation; there are no plots in the current figure, we do a plot (**new** is set to F), add lines, text or whatever is necessary; once we are finished with this particular plot we want to move to a new one. Since **new** is F we only need to call the high level function and it will start a new plot without overwriting the current one. In some circumstances we may want to overlay the results of two high level plotting functions. In this case we type **par(new=T)** before executing the second one and its output will be overlayed on top of the output of the first function. We will have more examples about this later.

A side effect of the way **new** operates is that when setting up the device layout, if there is more than one plot per page, the current figure is set to be the last one in the layout and **new** is set to **F**. This way, calling a high level plotting command will cause the device to move to the next figure in the layout, i.e. the first one, correctly producing the plot. The problem is that if we try to execute a *low level* plotting command, the results will apply to the last figure in the layout which is probably not what we intended.

12.1.6 A More Flexible Layout

Other parameters that change when setting mfrow or mfcol are fig and mfg. Notice that the mf* parameters divide the screen in regions of *the same size*. Additional flexibility is possible by using mfg and fig. In fact, setting one of mfrow or mfcol changes both of these. mfg allows under certain conditions to expand a particular plot to fill a whole row or a whole column. fig is much more flexible and permits creative arrangements of the different plots.

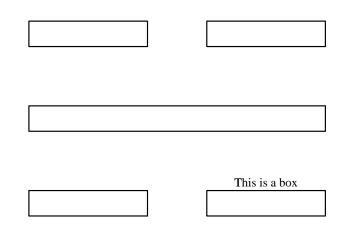


Figure 12.5: Flexible layout using mfg

The form of mfg is c(i,j,m,n), where i and j denote the row and column of the *current* figure in the multiple figure layout and m and n are the number of rows and columns. Thus, mfg can be used to make a specific figure active. The way to use mfg is to plan our layout and then after each plot change its value to make the next figure span a different region. For example

```
> par(mfg=c(1,1,3,2))
> box()
> par(mfg=c(1,2,3,2))
> box()
> par(mfg=c(2,1,3,1))
> box()
> par(mfg=c(3,1,3,2))
> box()
> par(mfg=c(3,2,3,2))
> box()
> title("This is a box")
```

The fig parameter allows greater flexibility than mfg. Simply set the coordinates of the figure region as a fraction of the device surface before each plot. The example above could have been

> par(fig=c(0,.5,.66,1))
> par(new=F)
> box()
> frame()
> par(fig=c(0,.5,.66,1))
> box()
> par(fig=c(.5,1,.66,1))
> box()
> par(fig=c(0,1,.33,.66))

> box()
> par(fig=c(0,0.5,0,.33))
> box()
> par(fig=c(0.5,1,0,.33))
> box()
> title("This is a box")

It is clear that by varying the parameters in fig we can obtain a much more flexible layout than by using mfg alone. A combination of both is most efficient, but setting fig will leave mfg unchanged. Also notice that the title function only affects the current figure. If we want to use an overall title we need to use mtext. There is an Hmisc function called mtitle which can also write an overall title. Look at it to see how it uses mtext.

12.1.7 Controlling Axes

With one exception, the parameters used to control the axes are all general parameters. That is, they can be changed as part of the argument to a high level plotting function, or through **par**. The exception is **axes** which is a high level parameter and can only be changed in the call to a high level plotting function. Using said parameters we can control four aspects of the axes: whether or not to draw an axis at all, the axis style (meaning, in general, the range), the style and positioning of labels, and length and position of tick marks.

We will now examine axes:

axes=L if FALSE, suppresses all axis plotting (x, y axes and box). Useful to make a high-level plotting routine generate only the plot portion of the figure.

If we choose to set this parameter to F, we may add a custom axis later by means of the axis function. It is also possible to eliminate the plotting of only one axis by using xaxt or yaxt. Setting either of these to "n" will produce that result. Other possibilities for these parameters are "s" (standard axis), "t" (time) and "l" (logarithmic).

The axis labels are modified through the parameters mgp, exp, lab and las. These are described below.

exp=x if exp=0, then axis labels in exponential notation have the "e" and the exponent on a newline. If exp is equal to 1, then such numbers are written all on one line. When exp=2 (the default), then numbers are written in the form 2*10^6.

lab=c(x,y,llen)

desired number of tick intervals on the x and y axes and the length of labels on both axes. The default is c(5,5,7).

las=x style of axis labels. 0 = always parallel to axis (the default), 1 = always horizontal, 2 = always perpendicular to axis.

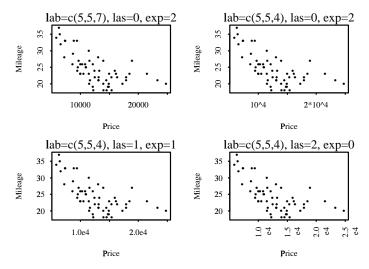


Figure 12.6: Controlling Axis Labels Style

```
mgp=c(x1,x2,x3)
```

margin line for the axis title, axis labels, and axis line in units of mex (see below). The default is c(3,1,0). Larger numbers are farther from the plot region, negative numbers are inside the plot region.

The next example from the car.test.frame dataframe illustrates the use of lab, las and exp.

```
> attach(car.test.frame)
> par(mfrow=c(2,2))
> plot(Price,Mileage,main="lab=c(5,5,7), las=0, exp=2")
> plot(Price,Mileage,main="lab=c(5,5,4), las=0, exp=2",
+ lab=c(5,5,4),las=0)
> plot(Price,Mileage,main="lab=c(5,5,4), las=1, exp=1",
+ lab=c(5,5,4),las=1,exp=1)
> plot(Price,Mileage,main="lab=c(5,5,4), las=2, exp=0",
+ lab=c(5,5,4),las=2,exp=0)
```

The mode of axis interval calculation can be controlled individually for the x and y axis by means of xaxs and yaxs. The value for these parameters can be any of "r", "i", "e", "s" or "d". A description of what they mean follows

xaxs="c" style of axis interval calculation. The styles "s" and "e" set up standard and extended axes, where numeric axis labels are more extreme than any data values. Extended axes may be extended another character width so that no data points lie very near the axis limit. Style "i" creates an axis labeled internal to the data values. This style wastes no space, yet still gives pretty labels. Style "r" extends the data range by 4% on each end, and then labels the axis internally. This ensures that all plots take up a fixed percent of the plot region, yet keeps points away from the axes. Style "d" is a direct axis, and axis parameters will not be changed by further high-level plotting routines. This is used to "lock-in" an axis from one plot to the next. The default is "r".

yaxs="c" see xaxs.

The most useful of these is style "d" which comes in handy when we want to overlay plots.

We already mentioned one of the parameters that control the number of tick marks, lab. They can also be controlled individually for each axis using xaxp and yaxp, but for this we need to set axes to F or xaxt or yaxt to "n" and then add the axes using axis. The length of tick marks is determined by tck which can also be used to put grids on the plot.

tck=x the length of tick marks as a fraction of the smaller of the width or height of the plotting region if less than one-half. When tck is more than one-half, the ticks are drawn across that fraction of the side; thus if tck equals 1, grid lines are drawn. If tck is negative, ticks are drawn outside of the plot region. The default is -.02.

```
xaxp=c(ul,uh,n)
```

coordinates of lower tick mark ul, upper tick mark uh, and number of intervals n within the range from ul to uh. For log axes if uh>1, uh is the number of decades covered plus 2 and n is the number of tick marks per decade (n may be 1, 2, or 9); if uh==1 then n is the upper tick mark. xaxp and yaxp are set by high level plotting functions, based on the current values in lab (and log) and used by the axis function (which is called implicitly by most high level plotting functions unless you use the argument axes=F).

yaxp=c(ul,uh,n) see xaxp.

Here's an example of different tck values.

```
> par(mfrow=c(2,2))
> plot(x,y,main="tck=-0.02")
> plot(x,y,main="tck=0.05",tck=0.05)
> plot(x,y,main="tck=1",tck=1)
> plot(x,y,yaxt="n",main="Different tick marks for each axis")
> axis(2,tck=1,lty=2)
```

The minor.tick function in Hmisc makes it easy to add tick marks for minor axis subdivisions.

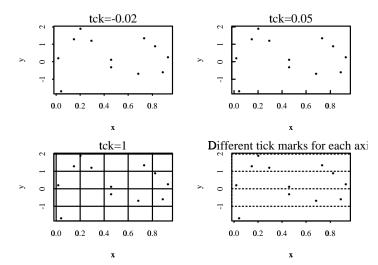


Figure 12.7: Examples of tick marks

12.1.8 Overlaying Figures

If we have a plot and we want to overlay different graphics elements on top of it, usually, the simplest way to do it is to use some low-level graphics functions such as lines or points. Other possibilities include arrows, symbols, abline, segments, matlines, matpoints, and, in the case of time-series plots, tslines and tspoints. These functions may not work if the new plot is on a different scale than the existing one. We have two main methods of dealing with this situation. One is to use a combination of the function axis and the parameter new, and the other is to use the function subplot. The latter one has other uses as well.

Let us examine in more detail the **axis** function. A section of the help file follows

```
Add an Axis to the Current Plot
DESCRIPTION:
    Adds an axis to the current plot. The side, positioning
    of tick marks, labels and other options can be specified.
USAGE:
    axis(side, at=<<see below>>, labels=T, ticks=T, distn=NULL, line=0,
    pos=<<see below>>, outer=F)
REQUIRED ARGUMENTS:
side: a number representing the side of the plot for the axis
    (1 for bottom, 2 for left, 3 for top, and 4 for right).
OPTIONAL ARGUMENTS:
at: vector of positions at which the ticks and tick labels
```

will be plotted. If side is 1 or 3, at represents xcoordinates. If side is 2 or 4, at represents ycoordinates. If at is omitted, the current axis (as specified by the xaxp or yaxp parameters, see par) will be plotted.

- labels: if labels is logical, it specifies whether or not to
 plot tick labels. Otherwise, labels must be the same
 length as at, and label[i] is plotted at coordinate at[i].
 ticks: if TRUE, tick marks and the axis line will be plotted.
- distn: character string describing the distribution used for transforming the axis labels. The only choice is distn="normal", in which case values of at are assumed to be probability levels, and the labels are actually plotted at qnorm(at). This also implies a reasonable default set of values for the at argument. By default the values in at are used as the labels.

. . .

Graphical parameters may also be supplied as arguments to this function (see par). However, arguments to title such as xlab and ylab are not allowed. For string rotation use the las graphical parameter: 0 = always parallel to the axis (the default), 1 = always horizontal to the axis, 2 =always perpendicular to the axis. The srt graphical parameter may be ignored for Windows.

This is a low-level plotting function (it adds an axis to the existing plot), and graphics parameters can be part of its argument. The only required argument is **side**, which indicates where the axis is going to be drawn, following the usual convention to denote the axes numbers. Most commonly, the **at** argument is used to specify the position of the tick marks, and the **labels** argument determines how they are going to be labeled. The labels justification and style are given by the parameters **srt** and **adj**. However, if **at** is not specified, then the values of **las** gives the orientation of labels. They will be centered at the tick mark if parallel to the axis, and right or left justified if perpendicular to it; left justified if inside the plot, right justified if outside, as determined by mgp. In this case **srt** and **adj** are ignored. Example

Notice that there is no box and the axis style is somewhat different from what we are used to see. The reason for the absence of a box is that we set **axes=F** in the call to plot, which not only suppressed the axes but also the box. If we wanted to have a box we may easily do so by typing **box()**. On the other hand, we may want to have the old axis style and no box. One quick and easy fix is to look at the values of **usr** and draw vertical lines using **abline**.

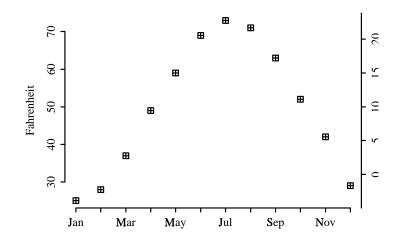


Figure 12.8: Use of axis

```
> par("usr")
[1] 0.56 12.44 23.08 74.92
> abline(v=0.56)
> abline(h=23.08)
```

If we want to be purists however, and get the right axes style from the beginning, we would just suppress the plotting of the x-axis by setting xaxs to "n" and change the box style with bty="l". The calls to axis as shown will give us the correct results.

Let us now use **axis** in combination with **xaxs** will also be handy here. We begin by changing the right margin to add space for an axis title there.

```
> par(mar=c(5,4,4,5)+.1)
> tsplot(hstart,ylab="Housing Starts")
```

Next we set par(new=T) in order not to erase the plot with a new call to tsplot and also par(xaxs="d") to retain the x-axis from the previous plot.

```
> par(new=T,xaxs="d")
> tsplot(ship,axes=F,lty=2)
> axis(side=4)
> mtext(side=4,line=3.8,"Manufacturing (millions of dollars)")
```

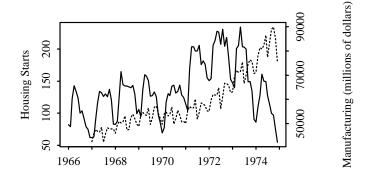
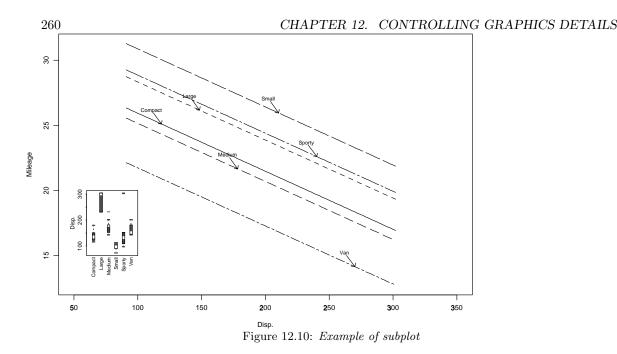


Figure 12.9: Overlaying high-level plots

The basic form of the subplot function is subplot(fun,x,y,size=c(1,1)). fun is any plotting routine that we want executed; x and y are the (user) coordinates of the current figure where the new plot will be positioned, and size is the size in inches of the new plot. subplot returns the values of the graphics parameters that were in effect for the subplot. For example, we could fit a least squares model in the car.test.frame and add a boxplot of the distribution of the predictors.

This plot allows to look at the distribution of Disp. by Type at the same time that examine their combined effect on Mileage.

More elaborate plots are possible using subplot. The next example adds graphical estimates of the density of Price and Mileage on top of a plot of Mileage vs Price.



> # Define the function using a logarithmic axes and plot the density
> subplot(x=c(.85,1),y=c(0,.85),fun=par(usr=c(0,1.04*max(den.m\$y),o.usr[3:4]));
+ lines(den.m\$y,den.m\$x);box()) # same here

In this example we have created a plot of Mileage vs Price using a logarithmic axis for the x-axis. We stored the value of the graphics parameters and later we stored the user coordinates of this plot (which was possible because we used subplot rather than plot). Then we created two lists with density estimates for Price and Mileage respectively. The next step is to plot these densities using subplot. Note that in the fun argument to subplot we are defining a function which changes the values of some parameters in the plot that subplot is going to create. The user coordinates y-axis range in the density plot of Price is is 4% bigger than the maximum value of the density estimate, and the x-axis range takes its values from the user coordinates from the first subplot. The xaxt parameter was set to "1" since the first plot also had a logarithmic x-axis. Something similar was done for the last subplot except that the roles of x and y had to be reversed.

12.2 Specifying a Graphical Output Device

Under UNIX, the printgraph function can be used to obtain a printed copy of the plot on the screen. In its simplest form, printgraph(), will send a copy of the plot on the screen to the default printer. This is equivalent to clicking on the print button of your current graphics device (usually openlook, motif, or win.graph). printgraph does not offer many options to control the printed output, and thus it does not provide any significant advantages over just clicking on the print button. In either UNIX or Windows you can use the dev.print function to print the current plot window or dev.copy to copy the current plot to a graphics file.

To effectively exercise control over aspects of your plot such as fonts and pointsize, you need to use a function appropriate to your printer or graphics editor. If you have a postscript printer, the

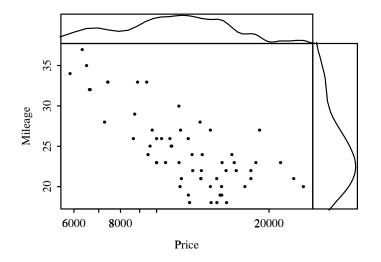


Figure 12.11: Another subplot example

function to use is postscript. For HP LaserJet printers you can use hplj, while for plotters using the HP-GL command set, the function to use is hpgl. To make a Windows metafile suitable for inclusion in Word or PowerPoint, you can use the format="placeable metafile" parameter with win.printer. Check the help for Devices for many more possibilities.

12.2.1 Opening Graphics Windows

In UNIX you usually open a graphics window with one of the following commands: openlook(), motif(), or X11(). In version 3.3 for Windows you can use win.graph or win.slide (see below), or gs.slide to set nice defaults for graph sheets in version 4.x.

12.2.2 The postscript, ps.slide, setps, setpdf Functions

There are many functions for specifying how graphics output can be stored in specially formatted graphics files. One of the most important functions is **postscript**, which works for both UNIX and Windows, although the **onefile** and **print.it** options do not apply to Windows.

```
> args(postscript)
function(file = NULL, width = -1, height = -1, append = F, onefile = T,
    print.it = NULL, ...)
```

When we type postscript(...), we open a graphics file in the same way that typing openlook opens a graphics device on the screen. The difference is that we will not be able to see the results until we close the postscript device and send the resulting postscript file to a printer or view the file with a postscript previewer. For this reason, it is advisable to create our plot in an openlook, motif, or win.graph device, and when we are satisfied with the results open a postscript device and repeat exactly the commands we used to get the plot in openlook. When we close thepostscript device

by typing dev.off() we will have a postscript file with our plot, or we may choose to send the output directly to the printer without saving the postscript file. It helps to keep all your plotting commands in a scratch file, that you may then copy and paste to your S-PLUS session window. For example, Fig. 12.10 was produced with the following commands.

Once you create a postscript graphics file you can preview it using Ghostview or other postscript previewers in UNIX or Windows.

Notice that the example uses an extra argument, pointsize that is not present in the list of arguments to postscript. The ... imply that other arguments are accepted. In UNIX (only), a list of all such arguments (including fonts), is available by typing ps.options().

The onefile=T argument means that successive plots will be acumulated in one file until we turn the device off. This may not be very useful if we want to incorporate the plots into a document. Setting onefile to F produces some peculiar results. In this case, each call to a high level plotting function will result in S sending all the plotting commands entered so far to the postscript file overwriting what was in it. To avoid this problem we must turn the device off before calling another high level plotting command. Another way around it is to omit the file argument and set print.it to F.

```
> postscript(onefile=F,print.it=F)
> plot(corn.rain)
> plot(corn.yield)
Starting to make postscript file.
Generated postscript file "ps.out.0001.ps".
> plot(corn.rain,corn.yield)
Starting to make postscript file.
Generated postscript file "ps.out.0002.ps".
> dev.off()
Starting to make postscript file.
Generated postscript file "ps.out.0003.ps".
```

The second call to plot closed the first postscript file; the third call closed the second file; to end with the third plot we had to close the device. This is just a way to produce several files with a single call to postscript. The reason for setting print.it to F is that, otherwise, S-PLUS would have printed the ps.out.* files and then deleted them. We could also have used a naming convention for the files.

```
> postscript(onefile=F,print.it=F,tempfile="corn.###.ps")
```

The **###** refer to a sequential number for the file name.

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The Hmisc ps.slide function for UNIX or Windows uses nice defaults to make four types of common postscript images, as controlled by an argument named type. Specify type=1 to make nice fullsize graphs or type=3 for making 5×7 " landscape graphs using 14-point type (useful for submitting to journals). type=2 (the default) is for color 35mm slides. Use type=4 to make nice black and white overhead projection transparancies (portrait mode). For example, use the following code for making a 5×7 " black and white graph with nice fonts.

```
ps.slide('myplot', type=3) # makes myplot.ps
plot(x, y)
dev.off()
```

See the online help for ps.slide for more options.

The Hmisc setps function makes small postscript figures suitable for papers. setps was used to produce the small graphs in this document¹. Here is an example.

setps also has an option to set up for trellis postscript graphics, and for converting postscript to .pdf. There is also an Hmisc function setpdf for setting up .pdf files, although creating a postscript file and converting it to .pdf often works better (as in the above example).

Windows users can easily incorporate postscript graphics into Microsoft Word and other applications (even though such graphics will not display on the screen) as long as they have a postscript printer.

12.2.3 The win.slide and gs.slide Functions

The basic plotting devices for Windows version 3.3 are win.graph and win.printer. To use nicer defaults for presentations and publications you can use the win.slide function in Hmisc. win.slide works similarly to ps.slide but draws graphs in the graphics window or writes a Windows metafile. If the file name is '', the graph is sent directly to the printer. The default value for type is 3 for win.slide. For S-PLUS version 4.x for Windows, you can use the Hmisc gs.slide function to set up nice defaults for graph sheets. When you copy graph sheets that have been produced with gs.slide in effect to the clipboard and paste the graphs into Microsoft applications, the results will be more pleasing than when using the default graphical parameters.

12.2.4 Inserting S Graphics into Microsoft Office Documents

In S-PLUS 2000 and S-PLUS 6, copying and pasting a graph sheet page into Microsoft Word, Powerpoint, etc. does not reliably render a graph. A more reliable approach is to do File ... Export Graph to explicitly export the graph into a Windows metafile. In Word you can insert the graph using Insert ... Picture ... From File. It is important not to resize or otherwise edit the

¹setps was changed to use a Helvetica font by default after these graphics were created.

graph using the mouse (for example by dragging a corner of the graph) as the graph will often become corrupted. To resize, right click and select a new size. To use a command to create a wmf file, use win.printer. In S-PLUS 6.0 (even under UNIX/Linux) you can use the wmf.graph function. Julian Wells has provided some valuable pointers for setting up graphics in Word:

Word 97 has good tools for explicit formatting of pictures: select the picture, then choose Format \rightarrow Picture (may show up as Format \rightarrow Object; this seems to depend on exactly what option one chose when inserting the picture with Paste \rightarrow Special). This brings up a tabbed dialogue box:

- The Picture tab allows you to crop the picture (so one can trim unwanted margins: there are also control here for colour, brightness and contrast, but I assume that scientific work will normally be black-and-white only)
- **The Size tab** allows one to change the size; the important thing here is that one has options to size relative to the original, and to maintain the original aspect ratio (the alternatives should be viewed very critically, in my opinion not keeping the aspect ratio will distort your favourite type face, for a start).

All this can be programmed simply by recording a macro, of course, so repetitive work is no problem.

The key thing in lining up the charts neatly is a good understanding of the use of the Word ruler and/or the Format \rightarrow Paragraph dialogue in line formatting (e.g. margins and indenting). I also find it very helpful to use table cells as containers for graphic material and captions – just about essential if one wants them in a multi-column layout.sent you.

Windows metafiles under the best of circumstances often do not render the graphic very well. The most beautiful graphs will be produced by outputting a postscript file for S and using Insert ... Picture in Word. This will put up a blank box on the screen but will print perfectly well to a postscript printer. If you want to be able to preview the graph on the screen (which is essential for Powerpoint presentations), have S-PLUS export the graph with a TIFF preview image. This will greatly enlarge the size of the graphics file, however.

Pstoedit is a useful program for converting postscript graphics files to a variety of formats (including windows metafiles) for editing and for importing into Micro Office. The Windows version of the program includes an Office graphics import plug-in for importing postscript graphics. pstoedit may be obtained at http://www.geocities.com/SiliconValley/Network/1958/pstoedit.

Chapter 13

Managing Batch Analyses, and Writing Your Own Functions

13.1 Using S in Batch Mode

As an exploratory tool it is best to use S interactively. Interactive use is also valuable for debugging a large S program. But it is useful to ultimately create a file which will have the main elements of the analysis and which we can submit at any point to obtain a final report. That way analyses can easily be updated when new data arrive, when data are corrected, or when additional analyses are desired.

In what follows, S-language source files have extension .s. If using the Windows S-PLUS script editor you might use its default suffix of .ssc. You can submit source files from inside S-PLUS to get the results on the screen, or use a batch command which will save the printed results to a file. See Section 1.5 for related material.

13.1.1 Batch Jobs in UNIX

Typing the following command at the UNIX prompt will cause S-PLUS to be run in batch mode in the background (omit the & to run it in the foreground):

```
Splus <file.s >file.lst &
```

This will run the S program file.s and produce the output file file.out.The command Splus BATCH file.s file.lst & is supposed to work but some users may have to prefix the command with nohup. It may be advantageous to define a UNIX shell program called Bs (in for example /usr/local/bin) to run S-PLUS jobs in the background at a low priority, causing input commands to be interspersed with the printed output. The shell (csh) program is defined as follows:

```
/bin/nice -5 Splus BATCH $1.s $1.lst
echo "echo "'pwd'"/$1.lst;tail "'$1' 'pwd'"/$1.lst" > $HOME/.lj
chmod a+x $HOME/.lj
```

Then you can initiate the job by typing Bs file at the UNIX prompt (note that the .s and & are implied automatically). Bs causes an executable program .lj to be placed in your root directory. When you enter the command .lj from any directory (assuming your home directory is in the directory path), the tail of the .lst file for the last job submitted will be printed. That makes it easy to monitor the job's progress.

Another useful script is Bsw, which causes the system to wait until the S-PLUS job is finished before running the next program. In some occasions you may have several files that need to be run in a given order; rather than doing one at a time you may create an executable file with a Bsw for all the files that need to be created and then have control returned to you after that file is executed. As an example suppose that we had edited a file create.all.s with all the S-PLUS jobs that need to be submitted. This master file might contain the following.

```
Bsw create.file1.s
    Bsw create.file2.s
              .
    Make it into an executable file (file owner only)
biostat3{cfa}: chmod u+x create.all.s
    Now run it
biostat3{cfa}: create.all.s &
   Bsw is defined as follows:
echo "echo "'pwd'"/$1.lst;tail "'$1' 'pwd'"/$1.lst" > $HOME/.lj
chmod +x $HOME/.lj
/bin/nice -5 echo 'options(echo=T)' | cat - $1.s | Splus 1>$1.lst 2>&1
The following is an example of a file you could submit.
   store()
   library(Design,T)
   postscript('/tmp/plot')
   . . . .
   plot(fit)
   # Define a function to print a heading with surrounding blank lines
   note \leftarrow function(text) cat('\n', text, '\n\n')
   note \leftarrow function(string) invisible(cat('\n', string, '\n\n'))
   note("time to dnr among pts with preference to forgo CPR")
   print(f)
```

```
print(anova(f))
```

We can run this code from inside S by typing source("filename.s") or src(filename), or in batch mode. Notice that we don't need quotes nor the ".s" extension with src. Apart from that the only difference is that src "remembers" the last file executed successfully, so, if you want to re-submit it, you need only type src().

13.1.2 Batch Jobs in Windows

As mentioned in Chapter 1, it is a good idea to make a shortcut to S-PLUS in each project directory. This will allow S-PLUS to be run interactively from that project directory. You can make a second shortcut for running S-PLUS in batch mode. For example, to run the program filename.s and create an output file filename.lst, use the Properties option in a shortcut to define a command such as c:\splus45\cmd\splus.exe S_PROJ=. /BATCH filename.s filename.lst filename.-log. Also, have the Start in box set to the project directory. Unfortunately, you'll have to edit the Properties or make a new shortcut for each source file to be used as the basis for a batch job.

To have your commands appear in the .lst file, put the command options(echo=T) at the start of the program or use the S_FIRST option below.

Assuming you are currently in the correct project directory, you can run S-PLUS from the DOS prompt using a command such as

start splus /BATCH my.s my.lst my.err S_PROJ=. S_FIRST='options(echo=T)'

To make DOS wait until S-PLUS finishes before running the next command, insert /w after start. To do the same thing in the Cygnus bash command shell under the Cygnus cygwin32 system, use a command like

/sp2000/cmd/splus.exe /BATCH my.s my.lst my.err S_PROJ=. S_FIRST='options(echo=T)'

Add & after the command to cause the system not to wait until S-PLUS finishes to go on to the next command.

You can run S-PLUS batch jobs from the Windows Start ...Run command by specifying a command such as splus /BATCH \mydir\prog.s \mydir\prog.lst S_PROJ=\mydir.

Using any of these approaches you will see a progress dialog. Add /BATCH_PROMPTS min to iconify this dialog.

The authoritative reference to the S-PLUS 2000 command line is S-PLUS 2000 Programmer's Guide, 1999, Chapter 19, which is available on the online help.

13.2 Managing S Non-Interactive Programs

As just discussed, an S program may easily be run in batch mode, producing a single .1st file containing the output. The batch program may also produce one or more plot files. However, in an analysis project it is frequently the case that some components of the analysis actually get completed, and if these require significant computer time, it is advantageous to not repeat those sub-analyses every time the program is run. Many analysts break down components of the analyses into a long array of batch programs which often contain highly repetitive setup code (e.g., recoding variables, extracting subsets of observations to process). Multiple programs can cause bookkeeping problems, so it is often better to keep related analysis steps in a single batch file. One can comment out sections of code that do not need to be executed again, it requires a significant amount of editing

to comment and un-comment large sections of code. A better approach is to make if statements apply to blocks of code:

This can be improved upon by making the program more self-documenting:

```
create \leftarrow F
fitmod \leftarrow F
valmod \leftarrow T
if(create) {
    df \leftarrow sas.get(...)
    df.desc describe(df)
    ddist \leftarrow datadist(df)
}
if(fitmod) {
    fit \leftarrow lrm(death \sim age*sex, x=T, y=T)
    print(fit)
    print(anova(fit))
}
if(valmod) {
    val \leftarrow validate(fit)
    print(val)
}
```

There are two disadvantages to the last two examples. First, you must explicitly print objects; typing fit instead of print(fit), for example, will not cause the object fit to print. This is because when you put a series of commands inside {}, the last object listed before the closing brace is "returned" by the nested expression, and only this last object is printed automatically. The second disadvantage is that the .lst file that was created when earlier parts of the program were executed will be overwritten by the new output.

The do function in Hmisc was created to facilitate conditional execution of parts of the analysis depending on what needs to be re-run. do makes it easy to write different parts of the analysis to different .lst files, and similarly it can segment plot output files. The first argument to do is a logical value. When this value is T, the second argument, which is an expression of arbitrary length, is executed. Otherwise this second argument is ignored. The second argument must be enclosed in {}; that is how it can contain multiple S statements. There are several optional arguments to do:

- device: This specifies a function that sets up the graphics device if any graphics are being done.
 do expects one of the following to be specified (in quotes): 'postscript', 'ps', 'ps.slide',
 'win.slide', 'win.printer'. device may also be specified through a system option called
 do.device, e.g., options(do.device = 'ps.slide').
- file: The name of the output file for this section of the program. It is automatically suffixed by .lst. file can be a special keyword 'condition', in which case the .lst file will be the

name of the first argument to do. file may also be specified through a system option called do.file.

append: Set this to T to have .lst output appended to an existing file.

- multiplot: Set this to T if you are using Windows and you wish each plot to go in a separate graphics file, with the files numbered sequentially.
- ... Any number of other arguments may be specified, which are passed to the plotting device function. For example, if using device='ps.slide'

Besides the system options mentioned above, selected system options work with do.

- do.prefix: A character string to prepend before .lst file names.
- do.echo: Type options(do.echo=F) to prevent S commands from being interspersed with function output in the .lst file.
- do.comments: Type options(do.comments=T) to include comments in the .lst file.

Here is an annotated example showing how to use this function. This example also shows how the Design library was used.

```
options(digits=3, datadist='ddist', continue='\n +',
        do.device='postscript', do.file='condition')
# do.file='condition' outputs do(condition,...) to condition.lst
# 'postscript' makes do(condition, ...) output postscript graphics
# into condition.ps
# May want to use do.device='win.slide' for Windows - uses nice defaults
# Add for example options(do.prefix='model') if you want .ps and .lst
# file names created by do() to be prefixed by 'model.' before any
# prefix normally created by do().
# Here is the analysis program, model.s
create
                     \leftarrow F
descriptives
                    \leftarrow F
ordinality
                    \leftarrow T
\texttt{cluster.fit.impute} \ \leftarrow \ \texttt{F}
                    \leftarrow F
full.model
                     \leftarrow \ F
find.penalty
\texttt{check.residuals} \quad \leftarrow \texttt{F}
separate.binary.fits \leftarrow F
                   \leftarrow T
validate.mod
simplify.nomogram \leftarrow T
do(create, {
  id='studyno', ifs='if chfdev>.')
  hist.data.frame(tami.chf, n.unique=2)
```

```
pstamp() # pstamp in Hmisc date-time stamps plots
 par(mfrow=c(4,5))
 plot(tami.chf[-c(2,4,5,9,11,12,16,18,19,21,22,24,25,26,27,28,32,36,37,38)],
      ask=F) # omit binary and ID vars
 pstamp()
 \leftarrow \texttt{datadist(tami.chf)}
 ddist
})
store()
attach(tami.chf)
table(chfdev)
table(newpe)
y <- score.binary(chfdev, newpe, death)
table(y)
table(y, yn)
# Could also use:
# y \leftarrow ifelse(death, 3, ifelse(newpe,2, ifelse(chfdev, 1, 0))) or
# y \leftarrow 0; y[chfdev==1] \leftarrow 1; y[newpe==1] \leftarrow 2; y[death==1] \leftarrow 3
do(ordinality, {
 summary(death \sim y.nodeath)
 par(mfrow=c(2,2))
 # The following is new:
 plot.xmean.ordinaly(y \sim age + efpre + izpre + numdz, cr=T)
 pstamp('Figure 1')
})
do(descriptives, {
 y3 \leftarrow cbind('>=CHF'=yn>=1, '>=PE'=yn>=2, Death=yn==3)
 # Stratify separately on each predictor variable, computing all
 # cumulative probabilities. For continuous variables, quartiles are used.
 s \leftarrow summary(y3 \sim age + cptrttim + diabp + sysbp + drug + efpre +
              eversmk + htn + hxdiab + hxsmk5 + izpre + miloc +
              nonizpre + numdz + ptca + pulse + pvd + race +
              ralesyn + s3 + sex, nmin=15)
 # Default summary function (fun=) is mean of each column of Y
 # Add ,fun='%' after nmin=15 to compute % instead of fractions
 w \leftarrow latex(s, longtable=T, title='descriptives') #makes descriptives.tex
```

```
# Instead, summarize using logits of cumulative probs.
 # qlogis is S's built-in log(p/(1-p)) function
 g \leftarrow function(y3) qlogis(c('Logit >=CHF'=mean(y3[,1]),
                            'Logit >=PE' =mean(y3[,2]),
                            'Logit Death'=mean(y3[,3])))
  s \leftarrow update(s, nmin=15, fun=g)
 # update -> do same summary as created previous s but change options
 # Make dot plots for first 11 of 21 predictor vars (too many for 1 page)
 cex.labels=.6, pch=c(5,10,183),
      pstamp('Figure 2') # date-time stamps lower right corner
  # Make dot plots for remaining variables
 plot(s[11:21,], which=1:3, xlab=xl, cex.labels=.6,
      pch=c(5,10,183), main=d)
 pstamp('Figure 3')
 logit \leftarrow function(p) ifelse(p==0 | p==1, NA, log(p/(1-p)))
  # qlogis did not work for next function - some conditional
  # probabilities were 0 and qlogis returned -infinity
 # logit is actually pre-defined (in /suserlib/.Data)
 h \leftarrow function(y) logit(c(mean(y==0), mean(y[y>=1]==1), mean(y[y>=2]==2)))
  s \leftarrow update(s, yn \sim ., fun=h) # same as previous s but with new fun
 plot(s[1:11,], which=1:3, xlab=xl \leftarrow 'Log Odds of Conditional Probability',
      cex.labels=.6, pch=c(5,10,183),
      main=d \leftarrow 'Examining Continuation Ratio Assumption')
 pstamp('Figure 4a')
 plot(s[11:21,], which=1:3, xlab=xl, cex.labels=.6,
      pch=c(5,10,183), main=d)
 pstamp('Figure 4b')
})
do(cluster.fit.impute, {
 par(mfrow=c(2,1))
 plot(naclus(tami.chf))
 pstamp('Figure 5')
 # Do hierarchical clustering based on a similarity matrix of
  # squared Spearman correlations
 vclus \leftarrow varclus(\sim.-studyno-race-tami-chfgrp-chf-timtohf-timtodth,
                  data=tami.chf, sim='spearman')
 store(vclus)
 plot(vclus)
 pstamp('Figure 6')
```

```
# Have transcan develop customized regression to predict each
 # predictor for all the other predictors. transcan will also
 # impute missing values. Use trantab=T so that fitted transformations
 # can be easily evaluated for future data
 trans \leftarrow transcan(\simage + cptrttim + diabp + efpre + eversmk + hbeta +
                  hcablock + htn + hxdiab + hxsmk5 + izpre + miloc +
                  murmur + nonizpre + numdz + ptca + pulse + pvd +
                  ralesyn + s3 + sex + sysbp + timi90,
                  imputed=T, shrink=T, trantab=T, eps=.5, pl=F)
 store(trans)
 par(mfrow=c(6,4))
 plot(trans)
 pstamp('Figure 7')
})
# Note how the following union of conditions makes it clear which
# parts of the analysis depend on the use of imputed values
do.impute.reduce \leftarrow full.model | find.penalty | check.residuals |
                  separate.binary.fits | simplify.nomogram
do(do.impute.reduce,
{
 # Imputation and data reduction needs to be done before any multivariable
 # model fits
 impute(trans) # imputes all variables, here putting them in .Data.tempxxxx
 describe(efpre)
 describe(efpre[is.imputed(efpre)])
 numdz \leftarrow round(numdz) # some imputed values were fractional
                      # since didn't tell transcan that
                      # numdz was categorical
          \leftarrow impute(drug) # replace 3 missing with most frequent (t-PA)
 drug
 table(race)
 # Combined last 5 levels of race
 levels(race) \leftarrow levels(race)[c(1,2,7,7,7,7,7)]
 # or levels(race) <- list(other=levels[3:7])</pre>
 table(race)
 map 
(2*diabp+sysbp)/3
 table(is.imputed(diabp),is.imputed(sysbp))
```

```
nrisk \leftarrow htn + pvd + hbeta + hcablock + murmur
 s3.rales \leftarrow s3 | ralesyn
 label(s3.rales) \leftarrow 'S3 Heart Sound or Rales'
 ddist \leftarrow datadist(ddist, map, race, nrisk, s3.rales, sex)
})
do(full.model,
 f \leftarrow lrm(y \sim rcs(age,3) + sex + race + rcs(map,4) + rcs(pulse,4) +
           pol(timi90,2) + rcs(izpre,4) + rcs(nonizpre,3) + rcs(efpre,3) +
           miloc + hxsmk5 + s3.rales + rcs(cptrttim,4) + ptca + drug +
           hxdiab + scored(numdz) + nrisk, x=T, y=T)
  f$stats
 prlatex(latex(f, caption='Full Unpenalized Nonlinear Model'))
 an \leftarrow anova(f)
 an
 plot(an)
 title('Strength of Predictors of Ordinal Response')
 pstamp('Figure 8')
 par(mar=c(5,4,4,5)+.1)
 plot(f, efpre=NA, ref.zero=T, ylim=c(-1.5,1.5))
 abline(h=0, lty=2)
 abline(v=medef \leftarrow ddist$limits$efpre[2], lty=2)
  axis(4, log(at \leftarrow c(.25, .5, .75, 1, 1.25, 1.5, 1.75, 2, 2.5, 3, 3.5, 4, 4.5)),
       labels=format(at), srt=90)
 mtext('Odds Ratio', side=4, line=3)
 text(medef, -1.3, 'Median efpre', adj=0, srt=90)
 title('Effect of efpre - Relative Log Odds')
 title(sub='plot(f, efpre=NA, ref.zero=T)', adj=0)
 pstamp('Figure 8a')
 par(mfrow=c(4,5), mar=c(5,4,4,1)+.1)
 plot(f, ref.zero=T, ylim=c(-1.5,1.5)) # no variables mentioned -> plot all
 # ref.zero=T -> Subtract a constant from X beta before plotting so
 # that the reference value of the x-variable yields y=0.
 pstamp('Figure 8b')
 store(f, 'fit.full')
})
options(do.file='condition')  # now make do() store results in sep. files
```

```
do(find.penalty, {
  # First try penalizing all parameters (except the intercept)
 # Try the following vector of penalty factors:
 pens \leftarrow c(1:10,20,40,80,160,320,640,1280,2500)
 pentrace(fit.full, pens)
 # Best penalty was 40, with 19.98 effective d.f. (AIC=147.1)
 # (Started with 34 d.f. in the unpenalized fit, AIC=133.5)
  # Now try penalizing only parameters associated with nonlinear effects
 pentrace(fit.full, pens, penalize=2)
 # Penalized model most likely to cross-validate the best is a model
 # with infinite penalty for the nonlinear terms (i.e., all betas for
 # nonlinear terms shrunk to zero).
 # This is consistent with the Wald statistics from
 # the combined nonlinear terms being 15.94 with 14 d.f., i.e., the
 # chi-sq is less than 28 -> further justification for using a linear
 # model. The model with no nonlinear terms has 20 d.f. and the
 # effective AIC in a 20.4 d.f. penalized model is 145, almost as good
 # as the 19.98 d.f. fully penalized nonlinear model.
 # Let's also fit a linear model and see if it could be improved on
 # by penalizing the linear effects. Let's cheat a little and use
  # prior knowledge on the ejection fraction transformation.
  f \leftarrow lrm(y \sim age + sex + race + map + pulse +
           timi90 + izpre + nonizpre + pmin(efpre,60) +
           miloc + hxsmk5 + s3.rales + cptrttim + ptca + drug +
           hxdiab + numdz + nrisk, x=T, y=T)
  f$stats
 prlatex(latex(f, caption='Full Unpenalized Linear Model'))
 anova(f)
  store(f, 'fit.full.linear')
 pt \leftarrow pentrace(f, pens)
 pt
 # We see that further shrinkage yields AIC=153 (with penalty=80, df=12.6)
 # Fit and save this penalized linear model
 f \leftarrow update(f, penalty=pt$penalty, x=T, y=T)
 prlatex(latex(f, caption='Full Penalized Linear Model'))
 anova(f)
 store(f, 'fit.full.linear.penalized')
})
```

do(check.residuals,

{

```
# Fit reduced model and check residuals on most important variables,
# to look for non-proportional odds. Also take a look at residuals
# from building block models used in continuation ratio model.
# Fast backward step-down, using default statistic (AIC) but
# Compute it on individual variables instead of using residual chi-square
# aics=0 means delete variables with AIC<2, AIC = chisq-2 x d.f.</pre>
# Override: do put map in model, and add hxsmk5 because of what was
# found later in the program.
fastbw(fit.full, type='individual', aics=2)
# Use untransformed predictors since we want to estimate transformations
# using partial residuals
f \leftarrow lrm(y \sim age + map + efpre + ptca + hxsmk5, x=T, y=T)
par(mfrow=c(2,3),oma=c(3,0,3,0))
resid(f, 'score.binary', pl=T)
mtitle('Binary Logistic Model Score Residuals\nFrom Ordinal Model Fit',
       ll='Figure 9')
# overall title+stamp, plus Figure # in lower left corner (11)
par(mfrow=c(2,3),oma=c(3,0,3,0))
resid(f, 'partial', pl=T)
mtitle('Binary Logistic Model Partial Residuals\nFrom Ordinal Model Fit',
       ll='Figure 10')
# Compute global goodness-of-fit statistics
# le Cessie - van Houwelingen - Hosmer (see residuals.lrm for refs)
resid(f, 'gof')
# Plot smoothed partial residuals for binary models that would be
# components of a forward continuation ratio model (temporarily
#combining 2 CHF categories).
fit.none \leftarrow lrm(yn==0 \sim age + map + efpre + ptca + hxsmk5, x=T, y=T)
fit.chf \leftarrow update(fit.none, yn==1 | yn==2 \sim ., subset=yn>=1)
fit.none$stats; fit.chf$stats
# The plot.lrm.partial function computes partial residuals for a
# sequence of binary logistic fits, and draws smoothed (lowess)
# partial residual plots for each predictor (all fits) on one graph.
# This is repeated for all predictors. See online help for residuals.lrm
par(mfrow=c(2,3), oma=c(3,0,3,0))
plot.lrm.partial(fit.none, fit.chf)
mtitle('Partial Residuals for 2 Binary Model Fits:\nY=0 and Y=1 or 2 | Y>0',
```

```
ll='Figure 11')
  # Do the same thing for backward continuation ratio models
  fit.death \leftarrow lrm(yn==3 \sim age + map + efpre + ptca + hxsmk5, x=T, y=T)
  fit.chf \leftarrow update(fit.death, yn==1 | yn==2 \sim ., subset=yn<3)
  fit.death$stats; fit.chf$stats
 par(mfrow=c(2,3), oma=c(3,0,3,0))
 plot.lrm.partial(fit.death, fit.chf)
 mtitle('Partial Residuals for 2 Binary Model Fits:\nY=3 and Y=1 or 2 \mid Y<3',
         ll='Figure 12')
})
do(separate.binary.fits,
{
  # Find list of variables that are important from either of 2
  # dichotomizations. Use linear models.
  # First, model for any CHF or death
  f.any \leftarrow update(fit.full.linear, yn>0 \sim ., x=F, y=F)
  fastbw(f.any, type='individual', aics=2)
  # Now model for death
  f.death \leftarrow update(f.any, yn==3 \sim ., x=T, y=T)
  f.death
  fastbw(f.death, type='individual', aics=2)
  # Demonstrate that if we wanted to develop a separate model for death,
  # significant shrinkage is needed since there are only 89 events
  pt \leftarrow pentrace(f.death, c(1,2,4,8,16,32,64,128,256))
 pt
  xbeta.orig \leftarrow predict(f.death)
  \texttt{f.death} \leftarrow \texttt{update(f.death, penalty=pt\$penalty, x=F, y=F)}
  # pt$penalty is best penalty as determined by pentrace (here, 32,
  # resulting in 11.7 effective d.f. - we started with 20 d.f.)
  f.death$stats
  # Compare predictive discrimination of customized death model
  # with ordinal model when asked to predict dead vs. alive
  somers2(predict(fit.full.linear.penalized), yn==3)
  plot(xbeta.orig, predict(f.death), ylab='Shrunken X*Beta', pch=202)
  # 202=small open circles (degree sign) on postscript printers
  abline(a=0, b=1, lwd=3)
```

```
title('Effect of Shrinkage on Linear Predictors\nIn Model for Death')
pstamp('Figure 13')
f.any \leftarrow lrm(yn>0 \sim age + map + pmin(efpre,60) + miloc + ptca +
           numdz + hxsmk5)
f.death \leftarrow update(f.any, yn==3 \sim .)
# Show side-by-side odds ratio charts. The the default (inter-quartile-
# range odds ratios) for continuous variables
s.any \leftarrow summary(f.any)
s.death \leftarrow summary(f.death)
par(mfrow=c(1,2), mgp=c(3,.4,0))
plot(s.any, log=T, main='Binary Model for Y>0',
    at = at \leftarrow c(.25,.5,1,2,4,8))
plot(s.death, log=T, main='Binary Model for Y=3', at=at)
pstamp('Figure 14')
# Fit a reduced ordinal model and compare the predictions it
# gives for Prob{death} to the predictions from f.death
f \leftarrow update(f.death, y \sim .)
prn(prob.death.ordinal[1:10,],
    'First 10 Rows of Reduced Ordinal Predictions')
describe(prob.death.ordinal - prob.death.customized)
par(mfrow=c(1,1))
plot(prob.death.ordinal, prob.death.customized, pch=202, log='xy',
    xlim=c(.001,.5),ylim=c(.001,.5))
abline(a=0, b=1, lwd=3)
scat1d(prob.death.ordinal)
scat1d(prob.death.customized, side=4)
title('Predicting Prob{Death} From\nCustomized and Proportional Odds Model')
# Form intervals of predicted probability of death from the ordinal
# model, such that there are 100 pts in each interval
# The levels.mean option to cut2 forces intervals to be labeled
# with the mean value within the interval, rather than the
# interval endpoints. This allows estimates to be positioned
# sensibly on the x-axis
# Now find 0.9 quantile of prob of death stratified by prob of
# death from ordinal model. Do same for 0.1 quantile.
```

```
upper \leftarrow tapply(prob.death.customized, pdo, quantile, probs=.9)
 # convert levels of stratification variable to numeric
 x ← as.numeric(levels(pdo))
                              # lty=2: dotted lwd=3: triple thickness
 lines(x, upper, lty=2, lwd=3)
 lines(x, lower, lty=2, lwd=3)
 pstamp('Figure 15')
})
do(validate.mod, {
 # Bootstrap validation of various indexes of fit
 val 
< validate(fit.full.linear.penalized, B=150)</pre>
 val
 store(val)
 # Bootstrap smooth (lowess) nonparametric calibration curve
 cal \leftarrow calibrate(fit.full.linear.penalized, B=150)
 store(cal)
 plot(cal)
 title('Bootstrap Calibration of Penalized Linear Model')
 pstamp('Figure 16')
 cal.unpen ← calibrate(fit.full.linear, B=150)
 store(cal.unpen)
 plot(cal.unpen)
 title('Bootstrap Calibration of Unpenalized Linear Model')
 pstamp('Figure 16b')
}, file='') # file='' -> print output goes to model.lst
do(simplify.nomogram, {
 # Approximate final model's predictions (logits) from a sub-model
 # This is more stable than doing stepwise variable selection against
 # the output, and it automatically makes use of penalization
 # Get predicted logit from final model (using first intercept)
 # Add a random error to this so that stepwise variable selection works
 f \leftarrow ols(alogit \sim age + sex + race + map + pulse +
          timi90 + izpre + nonizpre + pmin(efpre,60) +
          miloc + hxsmk5 + s3.rales + cptrttim + ptca + drug +
          hxdiab + numdz + nrisk)
 fastbw(f, aics=10000) # aics=10000: eventually delete all variables
 # Fit sub-model against final model's predicted logit, using last
 # few variables deleted by fastbw
```

```
f \leftarrow ols(plogit \sim pmin(efpre,60) + age + ptca + izpre + numdz +
          map + miloc + hxdiab + s3.rales)
  f
  # Compare approximate predicted logits to full model logits
  describe(abs(predict(f) - plogit))
  store(f, 'fit.full.linear.penalized.approx')
  # Make a nomogram based on the approximate model, with axes for
  # reading off predictions for all levels of output severity
  fun2 \leftarrow function(x) plogis(x-intercepts[1]+intercepts[2])
  fun3 \leftarrow function(x) plogis(x-intercepts[1]+intercepts[3])
 nomogram(f, fun=list('Prob(CHF or Death)'=plogis, 'Prob(PE or Death)'=fun2,
          'Prob(Death)'=fun3),
          fun.at=c(.01,.05,seq(.1,.9,by=.1),.95,.99),
          cex.var=.7, cex.axis=.75, lmgp=.2)
 pstamp('Figure 17')
}, file='')
print(scan('/users/feh/.lst', list(char.string='')), quote=F)
# .lst was created by do() if using UNIX (don't usually print this)
```

```
# can say .lst lpr to send all .lst files to printer, or .lst xless
# to view them all in windows. Do .lst ls to see their names.
# Note: The very first time .lst is created, the system won't
# be able to find it in your root directory unless it is the current
# directory. When you re-log in in the future, the system will
# note the existence of this executable file in your root area
# (you can issue the UNIX 'rehash' command to have .lst instantly
# available from any directory).
```

13.3 Reproducible Analysis

Common problems for an analyst are figuring out how she obtained a certain calculation, what subset of subjects was used to draw a graph, whether a regression analysis was run before or after a data error was corrected, and what sequence of menus was run to produce an analysis. These issues are especially important when formal inference is an important part of the analysis, and especially when results are submitted to a peer-reviewed journal or to a regulatory authority such as the FDA. We have worked with investigators who are completely unable to reproduce results they obtained using interactive software.

Even though interactive or exploratory analysis may be an ideal mode of operation for an FDA reviewer or anyone else wishing to review an analysis to check for robustness, interactive analysis does not lead to well-documented and easily re-run analyses. The best way to have reproducible analyses is to build a complete, cumulative script file as the analysis develops. This script file can be run as a batch file to produce a list or report file as well as several graphics files. Roger Koenker argues that the ultimate documentation of much of scientific research is the source code behind the production of calculations, plots, and tables, and such code (or a URL to it) should be included in many scientific publications.

But what if the analysis was split into several S jobs, and what if the analysis depended on an S data frame that was imported from a SAS dataset? If the SAS dataset were to be updated, how do we know what all needs to be re-run in S-PLUS? What if the graphics needed to be run through a command-oriented conversion program before inclusion in a report or on a Web page and we get tired of running the conversion steps manually? A solution to this problem is the use of the (originally) UNIX make utility program, also available on Linux and Windows 95/98/NT/2000 from the free Cygnus cygwin32 package from sourceware.cygnus.com/cygwin¹. In a Makefile you specify file dependencies. make analyzes these dependencies and examines file dates to see which programs need to be run so that all files are up to date.

Often in S-PLUS the final file to be produced is an object. Specifying an object name in .Data or _Data in your Makefile is no problem except that under Windows, S-PLUS still translates long file names to legal DOS names, and you will usually not know (or care about) such names. Possible solutions to this problem include creating as the final object in a job an object with a plain 8-letter (or less) name, or creating an ASCII file in the project directory (not in .Data) of any name. These "last objects created" can be used as the principal object name in the make dependencies.

As a demonstration of make under Windows, suppose we have the following files in our project directory:

```
test.dat
------
1 11
2 22
3 33
create.s
-------
dat <- read.table('test.dat',col.names=c('x','y'))
analyze.s
-------
library(Hmisc, T)
results <- describe(dat)</pre>
```

¹You have to install the full cygwin32 product to get make, i.e., full.exe, not usertools.exe. See biostat.mc. vanderbilt.edu/EmacsLaTeXTools for tips on installing cygwin32.

Makefile

```
Splus = /sp2000/cmd/splus.exe S_PROJ=. S_FIRST='options(echo=T)' /BATCH
DATA = ./_Data
.IGNORE:
.INIT:
all: $(DATA)/results $(DATA)/dat
$(DATA)/results: analyze.s $(DATA)/dat
$(Splus) analyze.s analyze.lst analyze.err
$(DATA)/dat: create.s test.dat
```

\$(Splus) create.s create.lst create.err

Note that in Makefile the indented lines have a tab, not spaces, on the left. To run the Makefile type make at the bash prompt. This will cause objects to be created if they don't already exist, or cause them to be re-created if their ancestors are deleted or modified.

A very nice tutoral on make by Duncan Temple Lang and Steve Golovich may be found in in an issue of the Statistical Computing and Graphics Newsletter at http://cm.bell-labs.com/cm/ms/who/cocteau/newsletter/issues/v92/v92.pdf.

Perl is a powerful language that is useful for a huge variety of tasks (such as manipulating data files) including managing program execution. In the example below for Unix/Linux, a directory named input_dir contains a list of input files to process, in a text file called List (one file name per line). An application called APP is run on each file to create a corresponding output file in directory output_dir. APP is only run when the input file has changed since the output file was last created, or if the corresponding output file does not exist. There is one exception. One of the file names in List needs to be changed. Also, the name of the output file is actually contained in the first line of the individual input file, after "# ", with a suffix of .ppp added.

```
#!/usr/bin/perl
$input_dir = "/home/mine/dir";
$output_dir = "/home/mine/otherdir";
open(LSTFILE,"$input_dir/List");
@files = <LSTFILE>;
foreach $file (@files) {
   chop $file; # remove end of line character
   # Exception for input file name: use yyyy instead of xxx for one file
   $file =~ s/xxx/yyyy/;
   $outfile = 'head -1 $input_dir/$file'; # Get 1st line
   # Note: command enclosed in back quotes: run UNIX command, return result
   chop $outfile;
   $outfile = substr($outfile, 2, 100); # Remove leading "# "
   $infile_age = (-M "$input_dir/$file"); # -M: modification age in days
```

```
$destfile = "$output_dir/$outfile.ppp";
if(fileolder($destfile,$infile_age)) {
    print "Converting $file \tto\t$destfile\n";
    system("cd $output_dir; APP < $input_dir/$file > $outfile.ppp;");
    }
  }
# Define a function that returns true if a file exists and is
# older than $age, or if the file does not exist
sub fileolder { #(filename, age)
    my($file, $age) = @_;
    (! ((-f $file) && ((-M $file) < $age)))
}
```

http://biostat.mc.vanderbilt.edu/StatReport has pointers to useful information about reproducible analysis.

13.4 Reproducible Reports

As it is relatively easy to specify S commands to produce ASCII files containing LATEX code, especially for tables, and it is very easy to produce postscript or pdf graphics files in an S program, running a master LATEX document containing \input statements that include LATEX code fragments or graphics files through the LATEX compiler will update the entire report, including cross-references, the table of contents, the index, etc. This LATEX step could easily be added to a Makefile such as the one above. See biostat.mc.vanderbilt.edu/StatReport/summary.pdf for detailed documentation for using S and LATEX to produce statistical graphical and tabular reports.

To assist in documenting how graphics are produced in a report, you can include the S code in the LATEX document after putting special comments in the code, e.g.

When the code is listed in the document, the actual figure number will be inserted in the S comment.

13.5 Writing Your Own Functions

13.5.1 Some Programming Commands

We will describe here the commands for loops and conditional execution of statements. In general, for dealing with structures such as matrices and vectors, it is preferable to use vectorized arithmetic and indexing rather than loops, but sometimes they are necessary.

The commands and their syntax are

| if(cond) expr | Evaluates <i>cond</i> ; if T evaluates <i>expr</i> |
|---|--|
| if(cond) expr1 else $expr2$ | Evaluates cond; if T evaluates expr1; if F evaluates expr2 |
| <pre>ifelse(cond,expr1,expr2)</pre> | This is a <i>vectorized</i> version of if else It evaluates |
| | cond and returns elements of expr1 for TRUE elements, |
| | and elements of $expr2$ for FALSE elements. |
| $\mathbf{switch}(expr,)$ | The result of <i>expr</i> must be character or numeric, it is compared |
| | to rest of the arguments and returns the first one that matches exactly. |
| for (name in expr1) expr2 | Evaluates $expr2$ for each name in $expr1$ |

13.5.2 Creating a New Function

One of the best features of S is perhaps the capability of writing your own functions. Most functions are written in the S language and you can look at them by just typing the function name

```
> sqrt
function(x)
x^0.5
```

Other functions are written in C or Fortran and you don't have easy access to them. However you can write a function that interfaces to a C or Fortran subroutine by using the functions .C and .Fortran. The general form of writing a function is

We can either create a text file with this code and submit it through a batch command such as Splus < filename.s or Bs filename in UNIX, or use the source or src functions or paste the function definition if operating in an interactive session. The function will then reside in your .Data directory unless you have something else attached in position one of the search list (same rules as with other objects apply).

The **bpower** function in Hmisc, which approximates the power of a two-sample binomial test, is a good example of a simple function that has a few options for how the calculations are done.

```
bpower \leftarrow function(p1, p2, odds.ratio, percent.reduction, n, n1, n2, alpha =0.05) {
    if(!missing(odds.ratio))
        p2 \leftarrow (p1 * odds.ratio)/(1 - p1 + p1 * odds.ratio)
    else if(!missing(percent.reduction))
        p2 \leftarrow p1 * (1 - percent.reduction/100)
    if(!missing(n)) {
        n1 \leftarrow n2 \leftarrow n/2
    }
    z \leftarrow qnorm(1 - alpha/2)
    q1 \leftarrow 1 - p1
    q2 \leftarrow 1 - p2
    pm \leftarrow (n1 * p1 + n2 * p2)/(n1 + n2)
```

```
\begin{array}{l} ds \ \leftarrow \ z \ * \ sqrt((1/n1 \ + \ 1/n2) \ * \ pm \ * \ (1 \ - \ pm)) \\ ex \ \leftarrow \ abs(p1 \ - \ p2) \\ sd \ \leftarrow \ sqrt((p1 \ * \ q1)/n1 \ + \ (p2 \ * \ q2)/n2) \\ c(Power \ = \ 1 \ - \ pnorm((ds \ - \ ex)/sd) \ + \ pnorm(( \ - \ ds \ - \ ex)/sd)) \\ \end{array}
```

Here is another simple function.

This function just calculates the Pearson correlation on the ranks of x and y after excluding missing values (since cor does not accept missing values).

We could build on the existing functions and write our own versions of them. We could issue the command

> my.matrix <-- edit(matrix)

to change the default parameter byrow from F to T. xedit will make an "edit" window with the code for matrix to appear and make the changes there. It is possible to use other editors. Others may use the function fix which works in a very similar way.

13.6 Customizing Your Environment

You can customize your S environment a little by defining a .First function. Here is an example:

The .First function contains commands that we want executed each time we start S-PLUS. For UNIX S-PLUS, If you want this function to be the same in all your subdirectories, you don't need to type it again. It is enough if you copy it to your .Data subdirectory. You can also have a .Last function as well. The store function in the Hmisc library creates a .Last function to delete temporary objects before S exits.

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